REMARKS

Claims 46 to 92 and 119 were objected to for containing "non-elected subject matter."

Claims 93 to 118 were withdrawn from consideration.

It was stated in the Office Action that claims 93 to 118 would be rejoined following allowability of claims 46 to 92 and 119, provided there are no problems under 35 USC 112.

Regarding the penultimate paragraph on page 2 of the Office Action, it is noted that on page 36, line 13 and page 37, line 8 of applicants' AMENDMENT UNDER 37 CFR 1.111 filed on May 17, 2005, it was intended that "MPEP 803.02" be cited.

In reply to applicants' species election for search purposes made in response to the November 19, 2004 Office Action, the Examiner examined a "subgeneric scope of the claims" as set forth on page 3 of the November 19, 2004 Office Action and withdrew from consideration the remaining subject matter included in claims 46 to 92. The "non-elected subject matter" referred to hereinabove is the claimed subject matter which is outside the scope of said "subgeneric scope of the claims." Actually, for the reasons discussed below, applicants never had the opportunity to make an election with regard to said "subgeneric scope of the claims."

Based on an election of species for search purposes only (in reply to the November 19, 2004 Office Action), the previous February 22, 2005 Office Action "jumped" to a restriction between a "Group (i)", namely R^1 and X^1 as defined in the claims; X^2 is oxygen; R^a as defined in the claims, but would not combine together with R^2 ; R^2 is H; R^3 is alkyl; A is $-C_2H_4-$; E is oxygen; and Arom is optionally substituted phenyl, and a "Group (ii)", namely the remainder of the claimed subject matter.

Prior to the November 19, 2004 Office Action, such purported restriction between said "Group (i)" and said "Group (ii)" had not previously been set forth as a Restriction Requirement under 35 USC 121, and applicants were not afforded an opportunity to elect and respond to said purported Restriction Requirement. The election between said "Group (i)" and said "Group (ii)" was in effect made for the applicants by the USPTO.

It is respectfully submitted that the previous February 22, 2005 Office Action did not establish a prima facie case for restricting the claims, because no reasons were furnished to justify restriction on the basis of any of (a) a separate classification, (b) a separate status of the art, or (c) a different field of search.

The Examiner is respectfully requested to follow the guidelines of MPEP 803.02 with respect to the elected species (for which no prior art is indicated as having been found) and to expand the examination to additional related species (for which it also appears that no prior art has been found) and continue the examination of the entire claimed subject matter.

Withdrawal of the Restriction Requirement which was set forth in the previous February 22, 2005 Office Action is respectfully requested for the following additional reasons.

The position is taken on page 3 of the June 17, 2005 Office action that the "substantial structural feature" in applicants' compounds is only a single ring with an amide substituent, and consequently running a search could "run the computer out of memory."

It is considered that the reason the Examiner does not see a complex substantial structural feature upon which to base his search is that the compounds in this case are structurally very simple. Furthermore, the range of substituents is very small. By incorporating the potential substituents into the search, it is respectfully submitted that the search is quite feasible and would not "run the computer out of memory," and consequently the first paragraph of MPEP 803.2 is appropriate.

Applicants have been able to run searches on these compounds and the results of such searches are submitted concomitantly herewith. The enclosed paper entitled "Search 1" relates to a search in which X^1 and X^2 were limited to oxygen.

Search 1 identified 94 documents, however, most compounds were in fact outside the scope of the claims, having, e.g., two ester groups on the phenyl ring, which is not permitted in claim 1. Additionally, many of these documents relate only to isolation of such di-substituted compounds from natural sources and with no apparent details of biological effects.

The enclosed two papers for Search 2 are split into the results from the CAS registry (no documents) and those from MARPAT (25).

The enclosed papers entitled "Search 2" relate to the following cases:

- (3) X^1 and X^2 are not both = 0
- (4) X¹ = O when X² = S
- (5) $X^1 = S \text{ when } X^2 = O$
- (6) Both X^1 and $X^2 = S$.

Search 2 identified 25 documents. Six of these post date the current application. No compounds falling within the scope of the claims were identified.

Also submitted concomitantly herewith are copies of the following papers concerning the corresponding European and International applications: the Supplementary European Search Report, the European Claims and the Translation of the International Preliminary Examination Report ("IPER").

In view of the above, withdrawal of the objection of claims 46 to 92 and examination of the entire scope of the claimed subject matter is respectfully requested.

Reconsideration is requested. Allowance is solicited.

An INFORMATION DISCLSOURE STATEMENT is being filed concomitantly herewith.

Appl. No. 10/629,108 Reply to Office Action dated June 17, 2005

If the Examiner has any comments, questions, objections or recommendations, the Examiner is invited to telephone the undersigned at the telephone number given below for prompt action.

Respectfully submitted,

Richard S. Barth Reg. No. 28,180

Frishauf, Holtz, Goodman & Chick, P.C. 220 Fifth Avenue - 16th Floor New York, New York 10001-7708 Tel. No. (212) 319-4900 Fax No. (212) 319-5101

E-mail Address: BARTH@FHGC-LAW.COM

RSB/ddf

Encs.: (1) INFORMATION DISCLOSURE STATEMENT

- (2) Copies of the following documents in the corresponding European and International application: Supplementary European Search Report, Translation of the International Preliminary Examination Report and the European claims
- (3) Search 1 (255 pages)
- (4) Search 2 CAS Registry (14 pages)
- (5) Search 2 MARPAT (111 pages)



SUPPLEMENTARY EUROPEAN SEARCH REPORT

Application Number EP 02 71 6323

Category	Citation of document with indicatio of relevant passages	n, where appropriate,	Relevant to claim	CLASSIFICATION OF THE APPLICATION (Int.CI.7)	
	No further relevant doci	uments disclosed		C07C219/30 C07C271/44 A61K31/137	
				TECHNICAL FIELDS SEARCHED (Int.Ci.7)	
				070	
	The supplementary search report has be set of claims valid and available at the s	een based on the last tart of the search.			
	Place of search MUNICH	Date of completion of the search	i	Examiner A	
X : part Y : part docu	ATEGORY OF CITED DOCUMENTS icularly relevant if taken alone icularly relevant if combined with another iment of the same category	T : theory or prin E : earlier patent after the filing D : document cit L : document cit	ciple underlying the document, but publy date ed in the application ed for other reasons	invention ished on, or	
A : technological background O : non-written disclosure P : Intermediate document		& : member of the same patent family, corresponding document			

Trainslation

PATENT COOPERATION TREATY

PCT

INTERNATIONAL PRELIMINARY EXAMINATION REPORT

(PCT Article 36 and Rule 70)

Applicant's or agent's file reference FP200201	FOR FURTHER ACTION		tionofTransmittalofInternational Preliminary n Report (Form PCT/IPEA/416)					
International application No.	International filing date (day)	month/year)	Priority date (day/month/year)					
PCT/JP02/00400	22 January 2002 (22	2.01.02)	26 January 2001 (26.01.01)					
	333/04, C07D 317/58, 317/6		3/63, 333/32, 333/40, 215/20, 209/44, 472, 4035, 55, A61P 43/00, 25/28, 24,					
Аррисан	SANKYO COMPANY	LIMITED						
and is transmitted to the applicant	according to Article 36.		national Preliminary Examining Authority					
2. This REPORT consists of a total of 3 sheets, including this cover sheet.								
amended and are the basis f 70.16 and Section 607 of th	for this report and/or sheets conta the Administrative Instructions un	ining rectifica	on, claims and/or drawings which have been ations made before this Authority (see Rule					
These annexes consist of a t	total of sheets.							
3. This report contains indications relating to the following items:								
Basis of the report								
II Priority	Delegates							
Non-astablishment	III Non-establishment of opinion with regard to novelty, inventive step and industrial applicability							
Peaconed statemen	Lack of unity of invention Reasoned statement under Article 35(2) with regard to novelty, inventive step or industrial applicability;							
citations and explanations supporting such statement EPO - DG 1								
VI Certain documents	cited							
VII Certain defects in t	the international application		0 3. 10. 2003					
VIII Certain observation	ns on the international application	n	109					
Date of submission of the demand		Date of completion of this report						
22 January 2002 (22.	01.02)	21 /	August 2002 (21.08.2002)					
Name and mailing address of the IPEA/JP	Autho	Authorized officer						
Faccimile No	Telan	hana Na						

International application No.

PCT/JP02/00400

INTERNATIONAL PRELIMINARY EXAMINATION REPORT

I. Basis	of the report
1. With	regard to the elements of the international application:*
	the international application as originally filed
	the description:
	pages, as originally filed
	pages , filed with the demand
	pages, filed with the letter of
	the claims:
	as originally files
	pages, as amended (together with any statement under Article 19
]	pages, filed with the demand
	pages, filed with the letter of
	the drawings:
	pages, as originally file
	pages, filed with the demand
	pages, filed with the letter of
	the sequence listing part of the description:
1	pages, as originally file
	pages, filed with the demand
	pages, filed with the letter of
the is	tregard to the language, all the elements marked above were available or furnished to this Authority in the language in which is neemational application was filed, unless otherwise indicated under this item. e elements were available or furnished to this Authority in the following language which is the language of a translation furnished for the purposes of international search (under Rule 23.1(b)). the language of publication of the international application (under Rule 48.3(b)). the language of the translation furnished for the purposes of international preliminary examination (under Rule 55.2 and
3. With	or 55.3). 1 regard to any nucleotide and/or amino acid sequence disclosed in the international application, the international minary examination was carried out on the basis of the sequence listing:
	contained in the international application in written form.
	filed together with the international application in computer readable form.
lĦ	furnished subsequently to this Authority in written form.
一片	furnished subsequently to this Authority in computer readable form.
	The statement that the subsequently furnished written sequence listing does not go beyond the disclosure in the international application as filed has been furnished.
	The statement that the information recorded in computer readable form is identical to the written sequence listing habeen furnished.
4.	The amendments have resulted in the cancellation of: the description, pages the claims, Nos the drawings, sheets/fig
5.	This report has been established as if (some of) the amendments had not been made, since they have been considered to g beyond the disclosure as filed, as indicated in the Supplemental Box (Rule 70.2(c)).**
in th	acement sheets which have been furnished to the receiving Office in response to an invitation under Article 14 are referred this report as "originally filed" and are not annexed to this report since they do not contain amendments (Rule 70.17).
1 ** Any .	replacement sheet containing such amendments must be referred to under item 1 and annexed to this report.

International application No.

INTERNATIONAL PRELIMINARY EXAMINATION REPORT

PCT/JP02/00400

tatement			
Novelty (N)	Claims	2-7, 16, 21-26, 29-31, 34-36	YE
	Claims	1, 8-15, 17-20, 27, 28, 32, 33	NO
Inventive step (IS)	Claims	2-7, 16, 21-26, 29-31, 34-36	YE
	Claims	1, 8-15, 17-20, 27, 28, 32, 33	NO
Industrial applicability (IA)	Claims	1-36	YE
	Claims		NO

2. Citations and explanations

Document 1: WO, 96-22276, A1 (Nippon Shinyaku Co., Ltd.), 25 July, 1996 (25.07.96), the claims, & AU, 9644589, A

Document 2: JP, 50-35175, A (Tanabe Seiyaku Co., Ltd.), 3 April, 1975 (03.04.75), the claims (Family: none)

The subject matters of claims 1, 8-13, 17-20, 27, 28, 32 and 33 do not appear to be novel or to involve an inventive step in view of document 1 cited in the ISR.

The compounds of the general formula (I) described in claim 1 and drugs containing any of the said compounds are disclosed in document 1.

The subject matters of claims 1, 14, 15, 19, 20, 27, 28 and 32 do not appear to be novel or to involve an inventive step in view of document 2 cited in the ISR.

The compounds of the general formula (I) described in claim 1 are disclosed in document 2.

The subject matters of claims 2-7, 16, 21-26, 29-31 and 34-36 appear to be novel and to involve an inventive step in view of documents 1 and 2 cited in the ISR.

Documents 1 and 2 do not describe that (a) the compounds of the general formula (I) having specific substituent groups and (b) the compounds of the general formula (I) have activity of inhibiting (a) acetylcholinesterase and (b) selective serotonin re-incorporation. This constitution is not considered to be obvious to a person skilled in the art either.

International application No.

PCT/JP02/00400

INTERNATIONAL PRELIMINARY EXAMINATION REPORT

Supplemental Box

(To be used when the space in any of the preceding boxes is not sufficient)

Continuation of:

IPC

C07D215/20, 209/44, 217/14, C07D217/16, 223/16, A61K31/27, A61K31/36, 31/44, 31/381, A61K31/47, 31/472, 31/4035, A61K31/55, A61P43/00, 25/28, A61P25/24, 25/14, 25/22 Claims:

25, 07, 2003

1. A compound of formula (I):



$$R^1$$
 X^2
 R^3
Arom
 R^3
 R^3

[wherein R^1 represents a C_1 - C_6 alkyl group, an amino group, a $(C_1$ - C_6 alkyl)amino group, a di $(C_1$ - C_6 alkyl)amino group or a nitrogen-containing saturated heterocyclic group;

 R^2 and R^3 are the same or different and represent a hydrogen atom or a $C_1\text{--}C_6$ alkyl group;

Arom represents an aryl group, an aryl group substituted at from 1 to 5 positions by substituent(s) which are the same or different selected from the substituent group α , a heteroaryl group, or a heteroaryl group substituted at from 1 to 3 positions by substituent(s) which are the same or different selected from the substituent group α ;

A represents a C1-C6 alkylene group;

 R^a represents a hydrogen atom, a C_1 - C_6 alkyl group or a C_1 - C_6 alkenyl group or, together with R^2 , represents a C_1 - C_3 alkylene group (in the case of C_2 - C_3 , it may contain a double bond);

E represents a single bond, an oxygen atom, a sulfur atom or a group of the formula: $-NR^4-$ (wherein R^4 represents a hydrogen atom or a C_1-C_7 alkanoyl group);

 X^1 and X^2 are the same or different and represent an oxygen atom or a sulfur atom] or a pharmacologically acceptable salt or ester thereof. <Substituent group α > halogen atom, C_1 - C_6 alkyl group, halogeno C_1 - C_6 alkyl group, C_1 - C_6 alkoxy group, C_1 - C_6 alkylthio group, C_1 - C_3 alkylenedioxy

- group, C_1 - C_7 alkanoyl group, C_2 - C_7 alkyloxycarbonyl group, amino group, C_1 - C_7 alkanoylamino group, hydroxyl group, mercapto group, cyano group, nitro group and carboxyl group.
- 2. A compound or pharmacologically acceptable salt or ester thereof according to Claim 1, wherein the group of formula: $R^1-C(=X^1)$ is a carbamoyl group, a $(C_1-C_4$ alkyl)carbamoyl group, a $di(C_1-C_4$ alkyl)carbamoyl group, a thiocarbamoyl group, a $(C_1-C_4$ alkyl)thiocarbamoyl group or a $di(C_1-C_4$ alkyl)thiocarbamoyl group.
- 3. A compound or pharmacologically acceptable salt or ester thereof according to Claim 1, wherein the group of formula: $R^1-C(=X^1)-\text{ is a }(C_1-C_4\text{ alkyl})\text{ carbamoyl group, a di}(C_1-C_4\text{ alkyl})\text{ carbamoyl group, a di}(C_1-C_4\text{ alkyl})\text{ thiocarbamoyl group or a di}(C_1-C_4\text{ alkyl})\text{ thiocarbamoyl group.}$
- 4. A compound or pharmacologically acceptable salt or ester thereof according to Claim 1, wherein the group of formula: $R^1-C(=X^1)$ is a $(C_1-C_4$ alkyl)carbamoyl group or a di $(C_1-C_4$ alkyl)carbamoyl group.
- 5. A compound or pharmacologically acceptable salt or ester thereof according to Claim 1, wherein the group of formula: $R^1-C(=X^1)$ is a di(C_1-C_4 alkyl)carbamoyl group.
- 6. A compound or pharmacologically acceptable salt or ester thereof according to Claim 1, wherein the group of formula: $R^1-C(=X^1)$ is a dimethylcarbamoyl group or an ethylmethylcarbamoyl group.
- 7. A compound or pharmacologically acceptable salt or ester thereof according to Claim 1, wherein the group of formula: $R^1-C(=X^1)$ is a dimethylcarbamoyl group,
- 8. A compound or pharmacologically acceptable salt or ester thereof according to any one of Claims 1 to 7, wherein R³ is a

C₁-C₆ alkyl group.

- 9. A compound or pharmacologically acceptable salt or ester thereof according to any one of Claims 1 to 7, wherein R³ is a methyl group or an ethyl group.
- 10. A compound or pharmacologically acceptable salt or ester thereof according to any one of Claims 1 to 7, wherein R^3 is a methyl group.
- 11. A compound or pharmacologically acceptable salt or ester thereof according to any one of Claims 1 to 10, wherein R^2 is a hydrogen atom or a C_1 - C_6 alkyl group.
- 12. A compound or pharmacologically acceptable salt or ester thereof according to any one of Claims 1 to 10, wherein R^2 is a hydrogen atom, a methyl group or an ethyl group.
- 13. A compound or pharmacologically acceptable salt or ester thereof according to any one of Claims 1 to 10, wherein R^2 is a hydrogen atom or a methyl group.
- 14. A compound or pharmacologically acceptable salt or ester thereof according to any one of Claims 1 to 10, wherein R^a , together with R^2 , is a C_1 - C_3 alkylene group which may contain a double bond.
- 15 A compound or pharmacologically acceptable salt or ester thereof according to any one of Claims 1 to 10, wherein R^a , together with R^2 , is a C_2 - C_3 alkylene group which may contain a double bond.
- 16. A compound or pharmacologically acceptable salt or ester thereof according to any one of Claims 1 to 10, wherein R^a , together with R^2 , is a C_3 alkylene group which contains a double bond.

- 17. A compound or pharmacologically acceptable salt or ester thereof according to any one of Claims 1 to 13, wherein R^a is a hydrogen atom or a methyl group.
- 18. A compound or pharmacologically acceptable salt or ester thereof according to any one of Claims 1 to 13, wherein R^a is a hydrogen atom.
- 19. A compound or pharmacologically acceptable salt or ester thereof according to any one of Claims 1 to 18, wherein Arom is a phenyl group, a phenyl group substituted at from 1 to 3 positions by substituent(s) which may be the same or different selected from the substituent group α , a pyridyl group, or a pyridyl group substituted at one position by a substituent selected from the substituent group α ;

<Substituent group α >

halogen atom, C_1 - C_6 alkyl group, halogeno C_1 - C_6 alkyl group, C_1 - C_6 alkoxy group, C_1 - C_6 alkylthio group, C_1 - C_3 alkylenedioxy group, C_1 - C_7 alkanoyl group, C_2 - C_7 alkyloxycarbonyl group, amino group, C_1 - C_7 alkanoylamino group, hydroxyl group, mercapto group, cyano group, nitro group and carboxyl group.

20. A compound or pharmacologically acceptable salt or ester thereof according to any one of Claims 1 to 18, wherein Arom is a phenyl group or a phenyl group substituted at from 1 to 3 positions by substituent(s) which may be the same or different selected from the substituent group α ;

<Substituent group α >

halogen atom, C_1 - C_6 alkyl group, halogeno C_1 - C_6 alkyl group, C_1 - C_6 alkoxy group, C_1 - C_6 alkylthio group, C_1 - C_3 alkylenedioxy group, C_1 - C_7 alkanoyl group, C_2 - C_7 alkyloxycarbonyl group, amino group, C_1 - C_7 alkanoylamino group, hydroxyl group, mercapto group, cyano group, nitro group and carboxyl group.

21. A compound or pharmacologically acceptable salt thereof according to any one of Claims 1 to 18, wherein Arom is a phenyl group substituted at one or two positions by

substituent(s) which may be the same or different selected from the substituent group $\alpha 1$, or a phenyl group substituted at three positions by halogen atoms;

<Substituent group α1>

halogen atom, C_1 - C_4 alkyl group, C_1 - C_4 alkyl group substituted by from 1 to 3 fluorine atoms, C_1 - C_4 alkoxy group, C_1 - C_4 alkylthio group, methylenedioxy group, ethylenedioxy group, C_1 - C_4 alkanoyl group, cyano group and nitro group.

- 22. A compound or pharmacologically acceptable salt thereof according to any one of Claims 1 to 18, wherein Arom is a phenyl group substituted at one or two positions by substituent(s) which may be the same or different selected from the substituent group $\alpha 2$, or a phenyl group substituted at three positions by fluorine atoms or chlorine atoms; <Substituent group $\alpha 2$ >
- fluorine atom, chlorine atom, methyl group, trifluoromethyl group, methoxy group, methylthio group, acetyl group, cyano group and nitro group.
- 23. A compound or pharmacologically acceptable salt thereof according to any one of Claims 1 to 18, wherein Arom is a phenyl group substituted at one or two positions by substituent(s) which may be the same or different selected from the substituent group $\alpha 3$, or a phenyl group substituted at three positions by fluorine atoms;

<Substituent group α3>

fluorine atom, chlorine atom, methylthio group, acetyl group, cyano group and nitro group.

24. A compound or pharmacologically acceptable salt thereof according to any one of Claims 1 to 18, wherein Arom is a phenyl group substituted at one or two positions by substituent(s) which may be the same or different selected from the substituent group $\alpha 4$, or a phenyl group substituted at three positions by fluorine atoms;

<Substituent group a4>

fluorine atom, chlorine atom, methylthio group and nitro group.

- 25. A compound or pharmacologically acceptable salt thereof according to any one of Claims 1 to 18, wherein Arom is a phenyl group substituted at one position by a fluorine atom, a chlorine atom or a nitro group, or a phenyl group substituted at two positions by fluorine atoms.
- 26. A compound or pharmacologically acceptable salt thereof according to any one of Claims 1 to 18, wherein Arom is a 4-fluorophenyl group, a 4-chlorophenyl group, a 4-nitrophenyl group or a 3,4-difluorophenyl group.
- 27. A compound or pharmacologically acceptable salt or ester thereof according to any one of Claims 1 to 26, wherein A is a C_1 - C_4 alkylene group.
- 28. A compound or pharmacologically acceptable salt or ester thereof according to any one of Claims 1 to 26, wherein A is a methylene group or an ethylene group.
- 29. A compound or pharmacologically acceptable salt or ester thereof according to any one of Claims 1 to 26, wherein A is an ethylene group.
- 30. A compound or pharmacologically acceptable salt or ester thereof according to any one of Claims 1 to 29, wherein E is an oxygen atom or a single bond.
- 31. A compound or pharmacologically acceptable salt or ester thereof according to any one of Claims 1 to 29, wherein E is an oxygen atom.
- 32. A compound or pharmacologically acceptable salt or ester thereof according to any one of Claims 1 to 31, wherein X^2 is an oxygen atom.

- 33. A pharmaceutical composition containing a compound or pharmacologically acceptable salt or ester thereof according to any one of Claims 1 to 32.
- 34. An inhibitor of acetylcholineesterase and selective serotonin reuptake containing a compound or pharmacologically acceptable salt or ester thereof according to any one of Claims 1 to 32.
- 35. A therapeutic or prophylactic drug for Alzheimer's disease, depression, Huntington's chorea, Pick's disease, tardive dyskinesia, compulsive disorders or panic disorders containing a compound or pharmacologically acceptable salt or ester thereof according to any one of Claims 1 to 32.
- 36. A therapeutic or prophylactic drug for Alzheimer's disease containing a compound or pharmacologically acceptable salt or ester thereof according to any one of Claims 1 to 32.

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L10
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L11
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L12
                STR
L13
                SCR 1842
L14 (
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L15 (
T.16
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     27 (Heterocyclic Compounds (One Hetero Atom))
     Tetrahydroisoquinolines. I. Formation and acid-catalyzed
rearrangement
     of 10-acetoxy-6-methoxy-2-methyl-7-oxo-\delta 5, 6, 8, 9-
     hexahydroisoquinolines
ST
     rearrangement acetoxy oxo isoquinoline
     Pomeranz-Fritsch reaction
        (of N-formyl-N-veratrylglycine)
IT
     Rearrangement
        (of acetoxymethoxymethyloxohexahydroisoquinoline derivs., mechanism
of
        acid-catalyzed)
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     450-14-6 19373-80-9 35005-99-3 35006-00-9
ΤT
                                                       35006-01-0
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TΨ
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        (oxidation by, of acetoxymethoxymethyloxohexahydroisoquinoline
derivs.)
     4876-18-0P
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                              19373-82-1P
                                              19373-83-2P
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     35006-11-2P
                   35006-12-3P
                                 35006-13-4P
                                               35035-02-0P 114139-18-3P
    RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
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HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

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=> d BIB HITSTR L16 1
THE ESTIMATED COST FOR THIS REQUEST IS 2.15 BRITISH POUNDS
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L16 ANSWER 1 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN
AN
     2003:728107 CAPLUS Full-text
DN
     140:128263
     A conformational restriction approach to the development of dual
     inhibitors of acetylcholinesterase and serotonin transporter as
potential
     agents for Alzheimer's disease
     Toda, Narihiro; Tago, Keiko; Marumoto, Shinji; Takami, Kazuko; Ori,
ΑU
     Mayuko; Yamada, Naho; Koyama, Kazuo; Naruto, Shunji; Abe, Kazumi;
     Yamazaki, Reina; Hara, Takao; Aoyagi, Atsushi; Abe, Yasuyuki; Kaneko,
     Tsugio; Kogen, Hiroshi
CS
     Exploratory Chemistry Research Laboratories, Sankyo Co., Ltd.,
     Shinagawa-ku, Tokyo, 140-8710, Japan
SO
     Bioorganic & Medicinal Chemistry (2003), 11(20), 4389-4415
     CODEN: BMECEP; ISSN: 0968-0896
PB
     Elsevier Science Ltd.
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     Journal
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     English
     444645-82-3P 444645-86-7P 444645-87-8P
     444645-89-0P 444645-94-7P 444645-96-9P
     444667-98-5P 649722-12-3P 649722-14-5P
     649722-16-7P 649722-18-9P 649722-21-4P
     649722-23-6P 649722-25-8P 649722-27-0P
     649722-29-2P 649722-31-6P 649722-33-8P
     649722-40-7P 649722-61-2P 649722-63-4P
     649722-67-8P 649722-69-0P 649722-71-4P
     649722-74-7P 649722-76-9P 649722-78-1P
     649722-80-5P 649722-82-7P 649722-84-9P
     649722-90-7P 649722-94-1P 649722-97-4P
     649723-00-2P 649723-04-6P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL
     (Biological study); PREP (Preparation)
        (preparation of dimethylcarbamic acid 2-methyl-1-[2-(4-
nitrophenoxy)ethyl]-
        2,3-dihydro-1H-benzo[c]azepin-7-yl ester and related compds. as
dual
        inhibitors of acetylcholinesterase and serotonin transporter)
RN
     444645-82-3 CAPLUS
CN
     Carbamic acid, dimethyl-, 1,2,3,4-tetrahydro-2-methyl-1-[2-(4-
     nitrophenoxy)ethyl]-6-isoquinolinyl ester, monohydrochloride (9CI)
(CA
     INDEX NAME)
```

HC1

RN 444645-86-7 CAPLUS

CN Carbamic acid, dimethyl-, 1-[2-(4-chlorophenoxy)ethyl]-1,2,3,4-tetrahydro-

2-methyl-7-isoquinolinyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} C1 \\ \\ CH_2 \\ \\ CH_2 \\ \\ CH_2 \\ \\ Me \end{array}$$

HCl

RN 444645-87-8 CAPLUS

CN Carbamic acid, dimethyl-, 2,3-dihydro-2-methyl-1-[2-(4-nitrophenoxy)ethyl]-

1H-2-benzazepin-7-yl ester, monohydrochloride (9CI) (CA INDEX NAME)

RN 444645-89-0 CAPLUS

CN Carbamic acid, dimethyl-, 1-[2-(4-chloro-3-methylphenoxy)ethyl]-2,3-dihydro-2-methyl-1H-2-benzazepin-7-yl ester, monohydrochloride (9CI)

(CA INDEX NAME)

RN 444645-94-7 CAPLUS

CN Carbamic acid, dimethyl-, (1S)-2,3-dihydro-2-methyl-1-[2-(4-nitrophenoxy)ethyl]-1H-2-benzazepin-7-yl ester, monohydrochloride (9CI)

(CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 444645-96-9 CAPLUS
CN Carbamic acid, dimethyl-, 1-[2-(4-chloro-3-methylphenoxy)ethyl]-2,3dihydro-2-methyl-1H-2-benzazepin-6-yl ester, monohydrochloride (9CI)
(CA
INDEX NAME)

RN 444667-98-5 CAPLUS
CN Carbamic acid, dimethyl-, (1R)-2,3-dihydro-2-methyl-1-[2-(4-nitrophenoxy)ethyl]-1H-2-benzazepin-7-yl ester, monohydrochloride
(9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

● HCl

RN 649722-12-3 CAPLUS
CN Carbamic acid, dimethyl-, 1,2,3,4-tetrahydro-1-[2-(4-nitrophenoxy)ethyl]-6isoquinolinyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Me 2N-

HCl

RN 649722-14-5 CAPLUS

CN Carbamic acid, dimethyl-, 1-[2-(4-chlorophenoxy)ethyl]-1,2,3,4-tetrahydro-

6-isoquinolinyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 649722-16-7 CAPLUS

CN Carbamic acid, dimethyl-, 1,2,3,4-tetrahydro-1-[2-(4-nitrophenoxy)ethyl]-7-

isoquinolinyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 649722-18-9 CAPLUS

CN Carbamic acid, dimethyl-, 1-[2-(4-chlorophenoxy)ethyl]-1,2,3,4-tetrahydro-

7-isoquinolinyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 649722-21-4 CAPLUS

CN Carbamic acid, dimethyl-, 1-[2-(4-chlorophenoxy)ethyl]-1,2,3,4-tetrahydro-

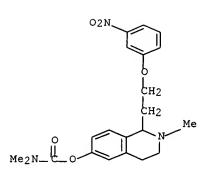
2-methyl-6-isoquinolinyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HCl

RN 649722-23-6 CAPLUS
CN Carbamic acid, dimethyl-, 1,2,3,4-tetrahydro-2-methyl-1-[2-(3-methyl-4nitrophenoxy)ethyl]-6-isoquinolinyl ester, monohydrochloride (9CI)
(CA
INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{Me} \\ \text{O} \\ \text{Me}_{2N-} \\ \text{O} \\ \text{O} \\ \text{Me}_{2N-} \\ \text{N} \\ \text{Me} \\ \text{Me}_{2N-} \\ \text{N} \\$$

● HCl



● HCl

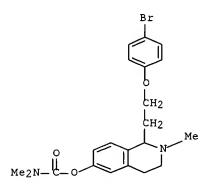
RN 649722-27-0 CAPLUS
CN Carbamic acid, dimethyl-, 1-[2-(4-fluorophenoxy)ethyl]-1,2,3,4tetrahydro2-methyl-6-isoquinolinyl ester, monohydrochloride (9CI) (CA INDEX
NAME)

● HCl

RN 649722-29-2 CAPLUS

CN Carbamic acid, dimethyl-, 1-[2-(4-bromophenoxy)ethyl]-1,2,3,4-tetrahydro-2-

methyl-6-isoquinolinyl ester, monohydrochloride (9CI) (CA INDEX NAME)



HC1

RN 649722-31-6 CAPLUS
CN Carbamic acid, dimethyl-, 1,2,3,4-tetrahydro-1-[2-(4-methoxyphenoxy)ethyl]2-methyl-6-isoquinolinyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 649722-61-2 CAPLUS
CN Carbamic acid, dimethyl-, 2,3-dihydro-1-[2-(4-nitrophenoxy)ethyl]-1H2benzazepin-7-yl ester, monohydrochloride (9CI) (CA INDEX NAME)

RN 649722-63-4 CAPLUS

CN Carbamic acid, dimethyl-, 1-[2-(4-chloro-3-methylphenoxy)ethyl]-2,3-dihydro-1H-2-benzazepin-7-yl ester, monohydrochloride (9CI) (CA INDEX NAME)

RN 649722-67-8 CAPLUS

CN Carbamic acid, dimethyl-, 1-[2-(4-chlorophenoxy)ethyl]-2,3-dihydro-2-methyl-1H-2-benzazepin-7-yl ester, monohydrochloride (9CI) (CA INDEX NAME)

RN 649722-69-0 CAPLUS

CN Carbamic acid, dimethyl-, 1-[2-(4-fluorophenoxy)ethyl]-2,3-dihydro-2-methyl-1H-2-benzazepin-7-yl ester, monohydrochloride (9CI) (CA INDEX NAME)

RN 649722-71-4 CAPLUS

CN Carbamic acid, dimethyl-, 2,3-dihydro-2-methyl-1-[2-[4-(trifluoromethyl)phenoxy]ethyl]-1H-2-benzazepin-7-yl ester, monohydrochloride (9CI) (CA INDEX NAME)

RN 649722-74-7 CAPLUS

CN Carbamic acid, dimethyl-, 2,3-dihydro-2-methyl-1-[2-(4-nitrophenoxy)ethyl]-

1H-2-benzazepin-8-yl ester, monohydrochloride (9CI) (CA INDEX NAME)

HCl

RN 649722-76-9 CAPLUS

CN Carbamic acid, dimethyl-, 1-[2-(4-chlorophenoxy)ethyl]-2,3-dihydro-2-methyl-1H-2-benzazepin-8-yl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 649722-78-1 CAPLUS

CN Carbamic acid, dimethyl-, 2,3,4,5-tetrahydro-1-[2-(4-nitrophenoxy)ethyl]-

1H-2-benzazepin-7-yl ester, monohydrochloride (9CI) (CA INDEX NAME)

RN 649722-80-5 CAPLUS

CN Carbamic acid, dimethyl-, 1-[2-(4-chlorophenoxy)ethyl]-2,3,4,5-tetrahydro-

1H-2-benzazepin-7-yl ester, monohydrochloride (9CI) (CA INDEX NAME)

RN 649722-82-7 CAPLUS

CN Carbamic acid, dimethyl-, 2,3,4,5-tetrahydro-2-methyl-1-[2-(4-nitrophenoxy)ethyl]-1H-2-benzazepin-7-yl ester, monohydrochloride (9CI)

(CA INDEX NAME)

RN 649722-84-9 CAPLUS
CN Carbamic acid, dimethyl-, 1-[2-(4-chlorophenoxy)ethyl]-2,3,4,5tetrahydro2-methyl-1H-2-benzazepin-7-yl ester, monohydrochloride (9CI) (CA
INDEX

NAME)

RN 649722-90-7 CAPLUS

CN Carbamic acid, dimethyl-, 2,3,4,5-tetrahydro-2-methyl-5-methylene-1-[2-(4- $\frac{1}{2}$

 $\label{lem:nitrophenoxy} \verb| ethyl] - 1 + 2 - benzazepin - 7 - yl ester, monohydrochloride (9CI)$

(CA INDEX NAME)

RN 649722-94-1 CAPLUS

(CA INDEX NAME)

RN 649722-97-4 CAPLUS

(CA INDEX NAME)

RN 649723-00-2 CAPLUS
CN Carbamic acid, dimethyl-, 2,3-dihydro-2-methyl-1-[2-(4-nitrophenoxy)ethyl]5-(2-thienyl)-1H-2-benzazepin-7-yl ester, monohydrochloride (9CI) (CA INDEX NAME)

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PAGE 2-A

NO2

HC1

```
IT
     474295-96-0P 474295-97-1P 474295-98-2P
     474295-99-3P 474296-00-9P 474296-01-0P
     474296-05-4P 474296-07-6P 649722-11-2P
     649722-13-4P 649722-15-6P 649722-17-8P
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     649722-89-4P 649722-91-8P 649722-92-9P
     649722-95-2P 649722-98-5P 649723-01-3P
     649723-02-4P 649723-07-9P 649723-08-0P
     649723-09-1P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT
     (Reactant or reagent)
        (preparation of dimethylcarbamic acid 2-methyl-1-[2-(4-
nitrophenoxy)ethyl]-
        2,3-dihydro-1H-benzo[c]azepin-7-yl ester and related compds. as
dual
        inhibitors of acetylcholinesterase and serotonin transporter)
     474295-96-0 CAPLUS
RN
     Carbamic acid, dimethyl-, 4-[(1R)-1-[[(1,1-
dimethylethoxy)carbonyl]amino]-
     3-(4-nitrophenoxy)propyl]-3-(methoxymethoxy)phenyl ester (9CI) (CA
INDEX
     NAME)
Absolute stereochemistry.
```

RN 474295-97-1 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1R)-1-[[(1,1-

dimethylethoxy)carbonyl]amino]-

3-(4-nitrophenoxy)propyl]-3-hydroxyphenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 474295-98-2 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1R)-1-[[(1,1-

dimethylethoxy)carbonyl]amino]-

3-(4-nitrophenoxy)propyl]-3-ethenylphenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

$$H_2C$$
 H_1N
 $OBu-t$
 NO_2
 Me_2N

RN 474295-99-3 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1R)-1-[[(1,1-dimethylethoxy)carbonyl]-2-propenylamino]-3-(4-nitrophenoxy)propyl]-3-ethenylphenyl ester (9CI)

(CA

INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 474296-00-9 CAPLUS
CN 2H-2-Benzazepine-2-carboxylic acid, 7-[[(dimethylamino)carbonyl]oxy]1,3dihydro-1-[2-(4-nitrophenoxy)ethyl]-, 1,1-dimethylethyl ester, (1R)(9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 474296-01-0 CAPLUS
CN Carbamic acid, dimethyl-, (1R)-2,3-dihydro-1-[2-(4-nitrophenoxy)ethyl]-1H2-benzazepin-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Absolute stereochemistry.

F₃C O HN OBu-t NO₂

RN 474296-07-6 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1R)-1-amino-3-(4-nitrophenoxy)propyl]-3-hydroxyphenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 649722-11-2 CAPLUS

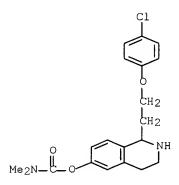
CN Carbamic acid, dimethyl-, 1,2,3,4-tetrahydro-1-[2-(4-nitrophenoxy)ethyl]-6-

isoquinolinyl ester (9CI) (CA INDEX NAME)

RN 649722-13-4 CAPLUS

CN Carbamic acid, dimethyl-, 1-[2-(4-chlorophenoxy)ethyl]-1,2,3,4-tetrahydro-

6-isoquinolinyl ester (9CI) (CA INDEX NAME)



RN 649722-15-6 CAPLUS
CN Carbamic acid, dimethyl-, 1,2,3,4-tetrahydro-1-[2-(4-nitrophenoxy)ethyl]-7isoquinolinyl ester (9CI) (CA INDEX NAME)

RN 649722-17-8 CAPLUS
CN Carbamic acid, dimethyl-, 1-[2-(4-chlorophenoxy)ethyl]-1,2,3,4-tetrahydro7-isoquinolinyl ester (9CI) (CA INDEX NAME)

RN 649722-86-1 CAPLUS
CN Carbamic acid, dimethyl-, 2,3,4,5-tetrahydro-1-[2-(4-nitrophenoxy)ethyl]-5-

oxo-1H-2-benzazepin-7-yl ester (9CI) (CA INDEX NAME)

RN 649722-87-2 CAPLUS

CN 2H-2-Benzazepine-2-carboxylic acid, 7-[[(dimethylamino)carbonyl]oxy]-1,3,4,5-tetrahydro-1-[2-(4-nitrophenoxy)ethyl]-5-oxo-, 1,1-dimethylethyl

ester (9CI) (CA INDEX NAME)

RN 649722-88-3 CAPLUS

CN 2H-2-Benzazepine-2-carboxylic acid, 7-[[(dimethylamino)carbonyl]oxy]1,3,4,5-tetrahydro-5-methylene-1-[2-(4-nitrophenoxy)ethyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 649722-89-4 CAPLUS
CN Carbamic acid, dimethyl-, 2,3,4,5-tetrahydro-2-methyl-5-methylene-1[2-(4nitrophenoxy)ethyl]-1H-2-benzazepin-7-yl ester (9CI) (CA INDEX NAME)

RN 649722-92-9 CAPLUS
CN 2H-2-Benzazepine-2-carboxylic acid, 7-[[(dimethylamino)carbonyl]oxy]1,3dihydro-5-methyl-1-[2-(4-nitrophenoxy)ethyl]-, 1,1-dimethylethyl ester
(9CI) (CA INDEX NAME)

RN 649722-95-2 CAPLUS
CN 2H-2-Benzazepine-2-carboxylic acid, 7-[[(dimethylamino)carbonyl]oxy]5ethenyl-1,3-dihydro-1-[2-(4-nitrophenoxy)ethyl]-, 1,1-dimethylethyl
ester
(9CI) (CA INDEX NAME)

RN 649722-98-5 CAPLUS
CN 2H-2-Benzazepine-2-carboxylic acid, 7-[[(dimethylamino)carbonyl]oxy]1,3dihydro-1-[2-(4-nitrophenoxy)ethyl]-5-(2-thienyl)-, 1.1-dimethylethyl

dihydro-1-[2-(4-nitrophenoxy)ethyl]-5-(2-thienyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 649723-01-3 CAPLUS
CN 2H-2-Benzazepine-2-carboxylic acid, 5-(4-chlorophenyl)-7[[(dimethylamino)carbonyl]oxy]-1,3-dihydro-1-[2-(4-

nitrophenoxy)ethyl]-,
 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

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NO2

RN 649723-02-4 CAPLUS

CN Carbamic acid, dimethyl-, 5-(4-chlorophenyl)-2,3-dihydro-1-[2-(4-nitrophenoxy)ethyl]-1H-2-benzazepin-7-yl ester (9CI) (CA INDEX NAME)

PAGE 1-A

NO2

RN 649723-08-0 CAPLUS
CN Carbamic acid, dimethyl-, 5-ethenyl-2,3-dihydro-1-[2-(4-nitrophenoxy)ethyl]-1H-2-benzazepin-7-yl ester (9CI) (CA INDEX NAME)

RN 649723-09-1 CAPLUS
CN Carbamic acid, dimethyl-, 2,3-dihydro-1-[2-(4-nitrophenoxy)ethyl]-5(2thienyl)-1H-2-benzazepin-7-yl ester (9CI) (CA INDEX NAME)

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474296-02-1P 649722-19-0P 649722-20-3P
IT
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     649722-77-0P 649722-79-2P 649722-81-6P
     649722-83-8P 649722-93-0P 649722-96-3P
     649722-99-6P 649723-03-5P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of dimethylcarbamic acid 2-methyl-1-[2-(4-
nitrophenoxy)ethyl]-
        2,3-dihydro-1H-benzo[c]azepin-7-yl ester and related compds. as
dual
        inhibitors of acetylcholinesterase and serotonin transporter)
     474296-02-1 CAPLUS
RN
     Carbamic acid, dimethyl-, (1R)-2,3-dihydro-2-methyl-1-[2-(4-
CN
     nitrophenoxy)ethyl]-1H-2-benzazepin-7-yl ester (9CI) (CA INDEX NAME)
```

Absolute stereochemistry. Rotation (-).

RN 649722-19-0 CAPLUS
CN Carbamic acid, dimethyl-, 1,2,3,4-tetrahydro-2-methyl-1-[2-(4-nitrophenoxy)ethyl]-6-isoquinolinyl ester (9CI) (CA INDEX NAME)

RN 649722-20-3 CAPLUS

CN Carbamic acid, dimethyl-, 1-[2-(4-chlorophenoxy)ethyl]-1,2,3,4-tetrahydro-

2-methyl-6-isoquinolinyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} C1 \\ CH_2 \\ CH_2 \\ CH_2 \\ \end{array}$$

$$Me_2N - \begin{array}{c} C \\ O \\ \end{array}$$

RN 649722-22-5 CAPLUS

CN Carbamic acid, dimethyl-, 1,2,3,4-tetrahydro-2-methyl-1-[2-(3-methyl-4-

nitrophenoxy)ethyl]-6-isoquinolinyl ester (9CI) (CA INDEX NAME)

RN 649722-24-7 CAPLUS

CN Carbamic acid, dimethyl-, 1,2,3,4-tetrahydro-2-methyl-1-[2-(3-nitrophenoxy)ethyl]-6-isoquinolinyl ester (9CI) (CA INDEX NAME)

RN 649722-26-9 CAPLUS

CN Carbamic acid, dimethyl-, 1-[2-(4-fluorophenoxy)ethyl]-1,2,3,4-tetrahydro-

2-methyl-6-isoquinolinyl ester (9CI) (CA INDEX NAME)

RN 649722-28-1 CAPLUS

CN Carbamic acid, dimethyl-, 1-[2-(4-bromophenoxy)ethyl]-1,2,3,4-tetrahydro-2-

methyl-6-isoquinolinyl ester (9CI) (CA INDEX NAME)

RN 649722-30-5 CAPLUS
CN Carbamic acid, dimethyl-, 1,2,3,4-tetrahydro-1-[2-(4-methoxyphenoxy)ethyl]2-methyl-6-isoquinolinyl ester (9CI) (CA INDEX NAME)

RN 649722-32-7 CAPLUS
CN Carbamic acid, dimethyl-, 1,2,3,4-tetrahydro-2-methyl-1-[2-(4-nitrophenoxy)ethyl]-7-isoquinolinyl ester (9CI) (CA INDEX NAME)

RN 649722-34-9 CAPLUS CN Carbamic acid, dimethyl-, 1-[2-(4-chlorophenoxy)ethyl]-1,2,3,4-tetrahydro-

2-methyl-7-isoquinolinyl ester (9CI) (CA INDEX NAME)

RN 649722-39-4 CAPLUS
CN Carbamic acid, dimethyl-, 1,2,3,4-tetrahydro-2-methyl-1-[2-(4-nitrophenoxy)ethyl]-5-isoquinolinyl ester (9CI) (CA INDEX NAME)

RN 649722-60-1 CAPLUS
CN Carbamic acid, dimethyl-, 2,3-dihydro-1-[2-(4-nitrophenoxy)ethyl]-1H2benzazepin-7-yl ester (9CI) (CA INDEX NAME)

RN 649722-62-3 CAPLUS

CN Carbamic acid, dimethyl-, 1-[2-(4-chloro-3-methylphenoxy)ethyl]-2,3-dihydro-1H-2-benzazepin-7-yl ester (9CI) (CA INDEX NAME)

RN 649722-64-5 CAPLUS

CN Carbamic acid, dimethyl-, 2,3-dihydro-2-methyl-1-[2-(4-nitrophenoxy)ethyl]-

1H-2-benzazepin-7-yl ester (9CI) (CA INDEX NAME)

RN 649722-65-6 CAPLUS

CN Carbamic acid, dimethyl-, 1-[2-(4-chloro-3-methylphenoxy)ethyl]-2,3-dihydro-2-methyl-1H-2-benzazepin-7-yl ester (9CI) (CA INDEX NAME)

RN 649722-66-7 CAPLUS

CN Carbamic acid, dimethyl-, 1-[2-(4-chlorophenoxy)ethyl]-2,3-dihydro-2-methyl-1H-2-benzazepin-7-yl ester (9CI) (CA INDEX NAME)

RN 649722-68-9 CAPLUS

CN Carbamic acid, dimethyl-, 1-[2-(4-fluorophenoxy)ethyl]-2,3-dihydro-2-methyl-1H-2-benzazepin-7-yl ester (9CI) (CA INDEX NAME)

RN 649722-70-3 CAPLUS

CN Carbamic acid, dimethyl-, 2,3-dihydro-2-methyl-1-[2-[4-(trifluoromethyl)phenoxy]ethyl]-1H-2-benzazepin-7-yl ester (9CI) (CA INDEX NAME)

RN 649722-72-5 CAPLUS

CN Carbamic acid, dimethyl-, 1-[2-(4-chloro-3-methylphenoxy)ethyl]-2,3-dihydro-2-methyl-1H-2-benzazepin-6-yl ester (9CI) (CA INDEX NAME)

RN 649722-73-6 CAPLUS

CN Carbamic acid, dimethyl-, 2,3-dihydro-2-methyl-1-[2-(4-nitrophenoxy)ethyl]-

1H-2-benzazepin-8-yl ester (9CI) (CA INDEX NAME)

RN 649722-75-8 CAPLUS

CN Carbamic acid, dimethyl-, 1-[2-(4-chlorophenoxy)ethyl]-2,3-dihydro-2-methyl-1H-2-benzazepin-8-yl ester (9CI) (CA INDEX NAME)

RN 649722-77-0 CAPLUS

CN Carbamic acid, dimethyl-, 2,3,4,5-tetrahydro-1-[2-(4-nitrophenoxy)ethyl]-

1H-2-benzazepin-7-yl ester (9CI) (CA INDEX NAME)

RN 649722-79-2 CAPLUS

CN Carbamic acid, dimethyl-, 1-[2-(4-chlorophenoxy)ethyl]-2,3,4,5-tetrahydro-

1H-2-benzazepin-7-yl ester (9CI) (CA INDEX NAME)

RN 649722-81-6 CAPLUS

CN Carbamic acid, dimethyl-, 2,3,4,5-tetrahydro-2-methyl-1-[2-(4-nitrophenoxy)ethyl]-1H-2-benzazepin-7-yl ester (9CI) (CA INDEX NAME)

RN 649722-83-8 CAPLUS

CN Carbamic acid, dimethyl-, 1-[2-(4-chlorophenoxy)ethyl]-2,3,4,5-tetrahydro-

2-methyl-1H-2-benzazepin-7-yl ester (9CI) (CA INDEX NAME)

RN 649722-93-0 CAPLUS
CN Carbamic acid, dimethyl-, 2,3-dihydro-2,5-dimethyl-1-[2-(4-nitrophenoxy)ethyl]-1H-2-benzazepin-7-yl ester (9CI) (CA INDEX NAME)

RN 649722-96-3 CAPLUS
CN Carbamic acid, dimethyl-, 5-ethenyl-2,3-dihydro-2-methyl-1-[2-(4-nitrophenoxy)ethyl]-1H-2-benzazepin-7-yl ester (9CI) (CA INDEX NAME)

649722-99-6 CAPLUS RN Carbamic acid, dimethyl-, 2,3-dihydro-2-methyl-1-[2-(4-CN nitrophenoxy)ethyl]-5-(2-thienyl)-1H-2-benzazepin-7-yl ester (9CI) (CA INDEX NAME)

649723-03-5 CAPLUS Carbamic acid, dimethyl-, 5-(4-chlorophenyl)-2,3-dihydro-2-methyl-1-CN [2-(4nitrophenoxy)ethyl]-1H-2-benzazepin-7-yl ester (9CI) (CA INDEX NAME)

PAGE 2-A

PAGE 1-A

NO2

THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT 26

ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d BIB HITSTR L16 2 THE ESTIMATED COST FOR THIS REQUEST IS 2.15 BRITISH POUNDS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y) /N: y L16 ANSWER 2 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN AN 2003:251390 CAPLUS Full-text DN 139:173164 Design, synthesis and structure-Activity relationships of dual TΙ inhibitors of acetylcholinesterase and serotonin transporter as potential agents for Alzheimer's disease Toda, Narihiro; Tago, Keiko; Marumoto, Shinji; Takami, Kazuko; Ori, ΑU Mayuko; Yamada, Naho; Koyama, Kazuo; Naruto, Shunji; Abe, Kazumi; Yamazaki, Reina; Hara, Takao; Aoyagi, Atsushi; Abe, Yasuyuki; Kaneko, Tsugio; Kogen, Hiroshi CS Exploratory Chemistry Research Laboratories, Sankyo Co., Ltd., Shinagawa-ku, Tokyo, 140-8710, Japan SO Bioorganic & Medicinal Chemistry (2003), 11(9), 1935-1955 CODEN: BMECEP; ISSN: 0968-0896 PB Elsevier Science Ltd. DТ Journal LA English 444644-04-6P 444644-05-7P 444644-06-8P 444644-07-9P 444644-08-0P 444644-13-7P 444644-14-8P 444644-15-9P 444644-26-2P 444644-36-4P 444644-44-4P 444644-49-9P 444644-52-4P 444644-62-6P 444644-63-7P 444644-85-3P 444644-90-0P 444645-11-8P 444645-12-9P 444645-16-3P 444645-31-2P 444645-32-3P 444645-47-0P 444645-58-3P 444667-96-3P 474295-89-1P 578729-98-3P 578729-99-4P 578730-07-1P 578730-08-2P 578730-09-3P 578730-10-6P 578730-16-2P 578730-17-3P 578730-18-4P 578730-19-5P 578730-20-8P 578730-21-9P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (design, synthesis and structure-Activity relationships of dual inhibitors of acetylcholinesterase and serotonin transporter as potential agents for Alzheimer's disease) RN444644-04-6 CAPLUS Carbamic acid, dimethyl-, 3-[1-(methylamino)-3-[4-CN (trifluoromethyl)phenoxy]propyl]phenyl ester, monohydrochloride (9CI) (CA

INDEX NAME)

HC1

RN 444644-05-7 CAPLUS
CN Carbamic acid, dimethyl-, 3-[3-(4-methoxyphenoxy)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HC1

RN 444644-06-8 CAPLUS
CN Carbamic acid, dimethyl-, 3-[1-(methylamino)-3-(4methylphenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HCl

RN 444644-07-9 CAPLUS
CN Carbamic acid, dimethyl-, 3-[3-(4-chlorophenoxy)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{NHMe} \\ \text{Me}_{2}\text{N} - \begin{array}{c} \text{Cl} \\ \text{CH} - \text{CH}_{2} - \text{CH}_{2} - \text{O} \end{array} \end{array}$$

● HCl

RN 444644-08-0 CAPLUS
CN Carbamic acid, dimethyl-, 3-[3-(4-fluorophenoxy)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX
NAME)

Me 2N - C - O CH - CH2 - CH2 - O F

HC1

RN 444644-13-7 CAPLUS
CN Carbamic acid, dimethyl-, 4-[3-(4-chlorophenoxy)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX
NAME)

HC1

HC1

RN 444644-15-9 CAPLUS
CN Carbamic acid, dimethyl-, 4-[3-(4-methoxyphenoxy)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 444644-26-2 CAPLUS

CN Carbamic acid, dimethyl-, 4-[3-(4-fluorophenoxy)-1-(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 444644-36-4 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(methylamino)-3-(4-methylphenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

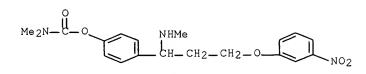
RN 444644-44-4 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(methylamino)-3-(4-nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HC1

RN 444644-49-9 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(methylamino)-3-(3-nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 444644-52-4 CAPLUS
CN Carbamic acid, dimethyl-, 4-[3-(4-cyanophenoxy)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me}_{2}\text{N} - \overset{\text{O}}{\text{C}} - \text{O} \\ \text{CH} - \text{CH}_{2} - \text{CH}_{2} - \text{O} \\ \end{array}$$

● HCl

RN 444644-62-6 CAPLUS
CN Carbamic acid, dimethyl-, 4-[1-(methylamino)-3-(2nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX
NAME)

● HCl

RN 444644-63-7 CAPLUS
CN Carbamic acid, dimethyl-, 4-[1-(methylamino)-3-phenoxypropyl]phenyl ester,
monohydrochloride (9CI) (CA INDEX NAME)

HCl

RN 444644-85-3 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(dimethylamino)-3-(4-nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 444644-90-0 CAPLUS

CN Carbamic acid, dimethyl-, 3-[1-(methylamino)-3-(4-nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HC1

RN 444645-11-8 CAPLUS
CN Carbamic acid, dimethyl-, 4-[1-(methylamino)-4-(4nitrophenoxy)butyl]phenyl ester, monohydrochloride (9CI) (CA INDEX
NAME)

HC1

RN 444645-12-9 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(methylamino)-2-(4-nitrophenoxy)ethyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me 2N-C-O} \\ \text{NHMe} \\ \text{CH-CH2-O} \end{array}$$

● HCl

RN 444645-16-3 CAPLUS
CN Carbamic acid, dimethyl-, 4-[1-(methylamino)-3-(4-nitrophenyl)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ Me\ 2N - C - O \\ \hline \\ CH - CH_2 - CH_2 \\ \hline \end{array}$$

HC1

RN 444645-31-2 CAPLUS
CN Carbamic acid, dimethyl-, 4-[1-(ethylamino)-3-(4nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX
NAME)

● HCl

RN 444645-32-3 CAPLUS
CN Carbamic acid, dimethyl-, 4-[1-(ethylmethylamino)-3-(4nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX
NAME)

HC1

RN 444645-47-0 CAPLUS
CN Carbamic acid, dimethyl-, 4-[1-(methylamino)-3-[(4nitrophenyl)thio]propyl]phenyl ester, monohydrochloride (9CI) (CA
INDEX

NAME)

$$\begin{array}{c} O \\ \text{Me 2N-C-O} \\ \hline \\ \text{CH-CH2-CH2-S} \\ \end{array}$$

● HCl

RN 444645-58-3 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1S)-3-(4-chlorophenoxy)-1-(methylamino)propyl]phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 444667-96-3 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1S)-1-(methylamino)-3-(4-nitrophenoxy)propyl]phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 474295-89-1 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1R)-1-(methylamino)-3-(4-nitrophenoxy)propyl]phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 578729-98-3 CAPLUS

CN Phenol, 4-[1-(methylamino)-3-(4-nitrophenoxy)propyl]-, methylcarbamate (ester), monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 578729-99-4 CAPLUS
CN Carbamic acid, ethyl-, 4-[1-(methylamino)-3-(4-nitrophenoxy)propyl]phenyl
ester, monohydrochloride (9CI) (CA INDEX NAME)

HC1

RN 578730-07-1 CAPLUS

CN Benzenemethanaminium, 4-[[(dimethylamino)carbonyl]oxy]-N,N,N-trimethyl-

 α -[2-(4-nitrophenoxy)ethyl]-, iodide (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ \text{Me 2N-C-O} \\ \hline \\ \text{CH-CH2-CH2-O} \end{array}$$

• I -

RN 578730-08-2 CAPLUS

CN Carbamic acid, dimethyl-, 4-[3-(4-nitrophenoxy)-1-(1-

pyrrolidinyl)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX
NAME)

RN 578730-09-3 CAPLUS
CN Carbamic acid, dimethyl-, 4-[3-(4-nitrophenoxy)-1-(1-piperazinyl)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$Me_{2}N - C - O \qquad NHMe \\ CH - CH_{2} - CH_{2} - NH - NO_{2}$$

HC1

578730-17-3 CAPLUS RN Carbamic acid, dimethyl-, 4-[3-[acetyl(4-nitrophenyl)amino]-1-(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HCl

578730-18-4 CAPLUS RNCarbamic acid, dimethyl-, 4-[1-(methylamino)-3-(4-CN nitrophenyl)propyl]phenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me2N-} \\ \text{C} \\ \text{C}$$

RN 578730-19-5 CAPLUS Carbamic acid, dimethyl-, 4-[3-(4-chlorophenoxy)-1-(methylamino)propyl]phenyl ester (9CI) (CA INDEX NAME)

578730-20-8 CAPLUS RN

Carbamic acid, dimethyl-, 4-[(1R)-3-(4-chlorophenoxy)-1-(methylamino)propyl]phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 578730-21-9 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(methylamino)-3-(4-nitrophenoxy)propyl]phenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me}_2\text{N} - \begin{array}{c} \text{O} \\ \text{O} \end{array} \\ \begin{array}{c} \text{NHMe} \\ \text{CH} - \text{CH}_2 - \text{CH}_2 - \text{O} \end{array} \\ \end{array}$$

RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d BIB HITSTR L16 3-94

THE ESTIMATED COST FOR THIS REQUEST IS 198.03 BRITISH POUNDS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y) /N:y

L16 ANSWER 3 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2003:163990 CAPLUS Full-text

DN 139:350659

TI Chemoselective oxidation of 3-acetyl-2,3-dihydrobenzothiazoles by dimethyldioxirane

AU Levai, Albert; Jeko, Jozsef

CS Department of Organic Chemistry, University of Debrecen, Debrecen, H-4010,

Hung.

SO ARKIVOC (Gainesville, FL, United States) (2003), (5), 19-27 CODEN: AGFUAR

URL: http://www.arkat-usa.org/ark/journal/2003/Bernath/GB-

642J/642J.pdf

PB Arkat USA Inc.

DT Journal; (online computer file)

LA English

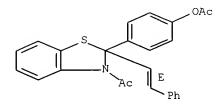
IT 191017-21-7 191017-23-9

RL: RCT (Reactant); RACT (Reactant or reagent)
(ring contraction of dihydrobenzothiazoles by acetic anhydride and
oxidation with dimethyldioxirane)

RN 191017-21-7 CAPLUS

CN Benzothiazole, 3-acetyl-2-[4-(acetyloxy)phenyl]-2,3-dihydro-2-[(1E)-2-phenylethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 191017-23-9 CAPLUS
CN Benzothiazole, 3-acetyl-2-[2-(acetyloxy)phenyl]-2,3-dihydro-2-[(1E)-2-phenylethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

IT 618113-97-6P 618114-01-5P 618114-02-6P 618114-03-7P 618114-04-8P 618114-05-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

RACT

(Reactant or reagent)

(ring contraction of dihydrobenzothiazoles by acetic anhydride and oxidation with dimethyldioxirane)

RN 618113-97-6 CAPLUS

CN Benzothiazole, 3-acetyl-2-[2-(acetyloxy)phenyl]-2,3-dihydro-2-[(1E)-2-

[4-

(1-methylethyl)phenyl]ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 618114-01-5 CAPLUS

CN Benzothiazole, 3-acetyl-2-[2-(acetyloxy)phenyl]-2-[(1E)-2-(3-chlorophenyl)ethenyl]-2,3-dihydro- (9CI) (CA INDEX NAME)

RN 618114-02-6 CAPLUS

CN Benzothiazole, 3-acetyl-2-[2-(acetyloxy)phenyl]-2-[(1E)-2-(4-chlorophenyl)ethenyl]-2,3-dihydro- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

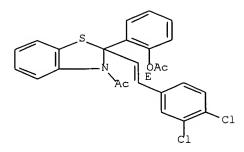
RN 618114-03-7 CAPLUS

CN Benzothiazole, 3-acetyl-2-[2-(acetyloxy)phenyl]-2-[(1E)-2-(2,4-dichlorophenyl)ethenyl]-2,3-dihydro- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 618114-04-8 CAPLUS

CN Benzothiazole, 3-acetyl-2-[2-(acetyloxy)phenyl]-2-[(1E)-2-(3,4-dichlorophenyl)ethenyl]-2,3-dihydro-(9CI) (CA INDEX NAME)



RN 618114-05-9 CAPLUS
CN Benzothiazole, 3-acetyl-2-[4-(acetyloxy)phenyl]-2-[(1E)-2-(4-chlorophenyl)ethenyl]-2,3-dihydro- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

Double bond geometry as shown.

RN 618113-99-8 CAPLUS
CN Benzothiazole, 3-acetyl-2-[2-(acetyloxy)phenyl]-2,3-dihydro-2-[(1E)-2-(3,4,5-trimethoxyphenyl)ethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 618114-00-4 CAPLUS

CN Benzothiazole, 3-acetyl-2-[2-(acetyloxy)phenyl]-2-[(1E)-2-(2-chlorophenyl)ethenyl]-2,3-dihydro-(9CI) (CA INDEX NAME)

Double bond geometry as shown.

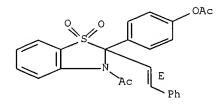
RN 618114-09-3 CAPLUS

CN Benzothiazole, 3-acetyl-2-[2-(acetyloxy)phenyl]-2,3-dihydro-2-[(1E)-2-phenylethenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 618114-10-6 CAPLUS

CN Benzothiazole, 3-acetyl-2-[4-(acetyloxy)phenyl]-2,3-dihydro-2-[(1E)-2-phenylethenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)



RN 618114-12-8 CAPLUS

CN Benzothiazole, 3-acetyl-2-[2-(acetyloxy)phenyl]-2,3-dihydro-2-[(1E)-2-

[4-

(1-methylethyl)phenyl]ethenyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 618114-13-9 CAPLUS

CN Benzothiazole, 3-acetyl-2-[2-(acetyloxy)phenyl]-2-[(1E)-2-(3-chlorophenyl)ethenyl]-2,3-dihydro-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 618114-14-0 CAPLUS

CN Benzothiazole, 3-acetyl-2-[2-(acetyloxy)phenyl]-2-[(1E)-2-(4-chlorophenyl)ethenyl]-2,3-dihydro-, 1,1-dioxide (9CI) (CA INDEX NAME)

RN 618114-15-1 CAPLUS
CN Benzothiazole, 3-acetyl-2-[2-(acetyloxy)phenyl]-2-[(1E)-2-(2,4-dichlorophenyl)ethenyl]-2,3-dihydro-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 618114-16-2 CAPLUS
CN Benzothiazole, 3-acetyl-2-[2-(acetyloxy)phenyl]-2-[(1E)-2-(3,4-dichlorophenyl)ethenyl]-2,3-dihydro-, 1,1-dioxide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 618114-17-3 CAPLUS
CN Benzothiazole, 3-acetyl-2-[4-(acetyloxy)phenyl]-2-[(1E)-2-(4-chlorophenyl)ethenyl]-2,3-dihydro-, 1,1-dioxide (9CI) (CA INDEX NAME)

OAC OAC

RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 4 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2002:667576 CAPLUS Full-text

DN 137:337771

TI Design and Synthesis of Dual Inhibitors of Acetylcholinesterase and Serotonin Transporter Targeting Potential Agents for Alzheimer's

Disease

AU Kogen, Hiroshi; Toda, Narihiro; Tago, Keiko; Marumoto, Shinji; Takami, Kazuko; Ori, Mayuko; Yamada, Naho; Koyama, Kazuo; Naruto, Shunji; Abe, Kazumi; Yamazaki, Reina; Hara, Takao; Aoyagi, Atsushi; Abe, Yasuyuki; Kaneko, Tsugio

CS Research Information Department, Exploratory Chemistry Research Laboratories, Neuroscience and Immunology Research Laboratories,

Sankyo

Co., Ltd., Shinagawa-ku, Tokyo, 140-8710, Japan

SO Organic Letters (2002), 4(20), 3359-3362

CODEN: ORLEF7; ISSN: 1523-7060

PB American Chemical Society

DT Journal

LA English

IT 474296-05-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

RACT

(Reactant or reagent)

(determination of absolute stereochem. of

(dimethylcarbamoyl) (nitrophenoxyethyl)ben

zylamine, prepared as dual acetylcholinesterase/serotonin transporter

inhibitor for Alzheimer's disease)

RN 474296-05-4 CAPLUS

CN Methanesulfonic acid, trifluoro-, 5-[[(dimethylamino)carbonyl]oxy]-2-[(1R)-

1-[[(1,1-dimethylethoxy)carbonyl]amino]-3-(4-

nitrophenoxy)propyl]phenyl
 ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 444644-93-3P 444667-98-5P 474295-89-1P 474296-03-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of chiral

(dimethylcarbamoyl) (nitrophenoxyethyl) benzylamine and

(dimethylcarbamoyl) (nitrophenoxyethyl) dihydrobenzazepine as dual acetylcholinesterase/serotonin transporter inhibitors for

Alzheimer's

disease)

RN 444644-93-3 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1S)-1-(methylamino)-3-(4-nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX

NAME)

Absolute stereochemistry.

HCl

RN 444667-98-5 CAPLUS

CN Carbamic acid, dimethyl-, (1R)-2,3-dihydro-2-methyl-1-[2-(4-nitrophenoxy)ethyl]-1H-2-benzazepin-7-yl ester, monohydrochloride (9CI)

(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

● HCl

RN 474295-89-1 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1R)-1-(methylamino)-3-(4-nitrophenoxy)propyl]phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

O₂N NHMe

RN 474296-03-2 CAPLUS
CN Carbamic acid, dimethyl-, (1S)-2,3-dihydro-2-methyl-1-[2-(4-nitrophenoxy)ethyl]-1H-2-benzazepin-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 474296-04-3

RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of chiral

(dimethylcarbamoyl) (nitrophenoxyethyl) benzylamine and

(dimethylcarbamoyl) (nitrophenoxyethyl) dihydrobenzazepine as dual acetylcholinesterase/serotonin transporter inhibitors for

Alzheimer's

disease)

RN 474296-04-3 CAPLUS

CN Carbamic acid, dimethyl-, (1S)-2,3-dihydro-1-[2-(4-

nitrophenoxy)ethyl]-1H-

2-benzazepin-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 444646-39-3P 444646-40-6P 444667-96-3P 474295-88-0P 474295-90-4P 474295-96-0P 474295-97-1P 474295-98-2P 474295-99-3P 474296-00-9P 474296-01-0P 474296-02-1P 474296-07-6P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of chiral (dimethylcarbamoyl) (nitrophenoxyethyl) benzylamine and

(dimethylcarbamoyl) (nitrophenoxyethyl) dihydrobenzazepine as dual acetylcholinesterase/serotonin transporter inhibitors for

Alzheimer's

disease)

RN 444646-39-3 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1S)-1-[[(1,1-

dimethylethoxy) carbonyl]methyla

mino]-3-(4-nitrophenoxy)propyl]phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 444646-40-6 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1R)-1-[(1,1-1)]

dimethylethoxy)carbonyl]amino]-

3-(4-nitrophenoxy)propyl]phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 444667-96-3 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1S)-1-(methylamino)-3-(4-nitrophenoxy)propyl]phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 474295-88-0 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1S)-1-[[(1,1-

dimethylethoxy)carbonyl]amino]-

3-(4-nitrophenoxy)propyl]phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 474295-90-4 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1R)-1-[[(1,1-

dimethylethoxy)carbonyl]methyla

mino]-3-(4-nitrophenoxy)propyl]phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 474295-96-0 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1R)-1-[[(1,1-

dimethylethoxy)carbonyl]amino]-

3-(4-nitrophenoxy)propyl]-3-(methoxymethoxy)phenyl ester (9CI) (CA INDEX

NAME)

Absolute stereochemistry.

RN 474295-97-1 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1R)-1-[[(1,1-

dimethylethoxy)carbonyl]amino]-

3-(4-nitrophenoxy)propyl]-3-hydroxyphenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN474295-98-2 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1R)-1-[[(1,1-

dimethylethoxy)carbonyl]amino]-

3-(4-nitrophenoxy)propyl]-3-ethenylphenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

$$H_2C$$
 H_1
 $OBu-t$
 NO_2
 Me_2N
 O

RN 474295-99-3 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1R)-1-[[(1,1-dimethylethoxy)carbonyl]-2propenylamino]-3-(4-nitrophenoxy)propyl]-3-ethenylphenyl ester (9CI)

(CA

INDEX NAME)

Absolute stereochemistry. Rotation (+).

474296-00-9 CAPLUS RN

2H-2-Benzazepine-2-carboxylic acid, 7-[[(dimethylamino)carbonyl]oxy]-CN1,3-

dihydro-1-[2-(4-nitrophenoxy)ethyl]-, 1,1-dimethylethyl ester, (1R)-(9CI)

(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 474296-01-0 CAPLUS
CN Carbamic acid, dimethyl-, (1R)-2,3-dihydro-1-[2-(4-nitrophenoxy)ethyl]-1H-

2-benzazepin-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 474296-02-1 CAPLUS

CN Carbamic acid, dimethyl-, (1R)-2,3-dihydro-2-methyl-1-[2-(4-nitrophenoxy)ethyl]-1H-2-benzazepin-7-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 474296-07-6 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1R)-1-amino-3-(4-nitrophenoxy)propyl]-3-hydroxyphenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

```
THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE.CNT 24
              ALL CITATIONS AVAILABLE IN THE RE FORMAT
L16 ANSWER 5 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN
     2002:575038 CAPLUS Full-text
DN
     137:140527
     Preparation of alkylcarbamic acid esters as acetylcholinesterase
TТ
inhibitor
     and serotonin reuptake inhibitor
     Koyama, Kazuo; Marumoto, Shinji; Toda, Narihiro; Kogen, Hiroshi;
Suzuki,
     Keiko
     Sankyo Company, Limited, Japan
PA
     PCT Int. Appl., 300 pp.
     CODEN: PIXXD2
DT
     Patent
LA
     Japanese
FAN.CNT 1
                                           APPLICATION NO. DATE
                      KIND DATE
     PATENT NO.
                     ----
                                          WO 2002-JP400
                                                            20020122
                            20020801
     WO 2002059074
                     A1
PΙ
         W: AU, BR, CA, CN, CO, CZ, HU, ID, IL, IN, KR, MX, NO, NZ, PH,
PL,
             RU, SG, SK, US, VN, ZA
         RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC,
NL,
             PT, SE, TR
                                                            20020122
     EP 1362844
                       A1
                            20031119
                                           EP 2002-716323
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC,
PT,
             IE, FI, CY, TR
                                           JP 2002-15136
                                                            20020124
     JP 2003176256
                      A2
                            20030624
PRAI JP 2001-18386
                       Α
                            20010126
     JP 2001-305182
                            20011001
                       Α
     WO 2002-JP400
                            20020122
                       W
     MARPAT 137:140527
OS
     444643-92-9P 444644-03-5P 444644-07-9P
     444644-26-2P 444644-76-2P 444644-78-4P
     444644-93-3P 444645-18-5P 444645-22-1P
     444645-29-8P 444645-33-4P 444645-35-6P
     444645-37-8P 444645-38-9P 444645-40-3P
     444645-41-4P 444645-45-8P 444645-47-0P
     444645-49-2P 444645-51-6P 444645-54-9P
     444645-56-1P 444645-62-9P 444645-64-1P
     444645-66-3P 444645-69-6P 444645-73-2P
     444645-78-7P
     RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
     preparation); THU (Therapeutic use); BIOL (Biological study); PREP
     (Preparation); RACT (Reactant or reagent); USES (Uses)
        (preparation of alkylcarbamic acid esters as acetylcholinesterase
inhibitor)
RN
     444643-92-9 CAPLUS
     Carbamic acid, dimethyl-, 3-[3-(4-methoxyphenyl)-1-
     (methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX
NAME)
```

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$$\begin{array}{c} \text{O} \\ \text{Me} \, 2\text{N} - \text{C} - \text{O} \end{array} \begin{array}{c} \text{N} \, \text{HMe} \\ \text{C} \, \text{H} - \, \text{C} \, \text{H} \, 2 - \, \text{C} \, \text{H} \, 2 \end{array}$$

● HCl

RN 444644-03-5 CAPLUS
CN Carbamic acid, ethyl-, 3-[3-(4-methoxyphenyl)-1(methylamino)propyl]phenyl
 ester, monohydrochloride (9CI) (CA INDEX NAME)

HCl

RN 444644-07-9 CAPLUS
CN Carbamic acid, dimethyl-, 3-[3-(4-chlorophenoxy)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX

$$\begin{array}{c} \text{O} \\ \text{Me}_2\text{N} - \begin{array}{c} \text{O} \\ \text{CH} - \text{CH}_2 - \text{CH}_2 - \text{O} \end{array} \end{array}$$

HC1

RN 444644-26-2 CAPLUS

NAME)

CN Carbamic acid, dimethyl-, 4-[3-(4-fluorophenoxy)-1- (methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HC1

RN 444644-76-2 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(methylamino)-3-(3,4,5-trifluorophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA

INDEX

NAME)

$$\begin{array}{c} \text{Me}_2\text{N} - \overset{\text{O}}{\text{C}} - \text{O} \\ \text{O} \\ \text{CH-CH}_2 - \text{CH}_2 - \text{O} \\ \end{array}$$

HC1

RN 444644-78-4 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1S)-3-(4-chlorophenoxy)-1- (methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

HCl

RN 444644-93-3 CAPLUS

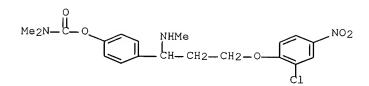
CN Carbamic acid, dimethyl-, 4-[(1S)-1-(methylamino)-3-(4-nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 444645-18-5 CAPLUS

CN Carbamic acid, dimethyl-, 4-[3-(2-chloro-4-nitrophenoxy)-1- (methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

Absolute stereochemistry.

HCl

Absolute stereochemistry.

● HCl

RN 444645-33-4 CAPLUS
CN Carbamic acid, dimethyl-, 4-[3-(4-chlorophenoxy)-1(ethylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

444645-35-6 CAPLUS RNCarbamic acid, dimethyl-, 4-[3-(3,4-difluorophenoxy)-1-

(ethylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX

NAME)

$$\begin{array}{c} \text{Me}_2\text{N} - \overset{\text{O}}{\text{C}} - \text{O} \\ & \text{CH} - \text{CH}_2 - \text{CH}_2 - \text{O} \end{array}$$

HC1

444645-37-8 CAPLUS RN

CN Carbamic acid, dimethyl-, 4-[1-(ethylmethylamino)-3-(4fluorophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

444645-38-9 CAPLUS RN

Carbamic acid, dimethyl-, 3-[3-(3-chlorophenoxy)-1-(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{NHMe} \\ \text{Me}_{2}\text{N} - \text{C}_{-0} \end{array} \\ \begin{array}{c} \text{NHMe} \\ \text{CH} - \text{CH}_{2} - \text{CH}_{2} - \text{O} \end{array}$$

● HCl

444645-40-3 CAPLUS

CN Carbamic acid, dimethyl-, 3-[3-(3-chloro-4-fluorophenoxy)-1- (methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HC1

RN 444645-41-4 CAPLUS
CN Carbamic acid, dimethyl-, 3-[3-(4-chloro-3-fluorophenoxy)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{NHMe} \\ \text{Me} \, 2\text{N} - \begin{array}{c} \text{O} \\ \text{CH} - \text{CH} \, 2 - \text{CH} \, 2 - \text{O} \end{array} \end{array}$$

HC1

RN 444645-45-8 CAPLUS
CN Carbamic acid, dimethyl-, 4-[(1R)-3-(3,4-difluorophenoxy)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 444645-47-0 CAPLUS
CN Carbamic acid, dimethyl-, 4-[1-(methylamino)-3-[(4-nitrophenyl)thio]propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HC1

RN 444645-49-2 CAPLUS
CN Carbamic acid, dimethyl-, 4-[3-[(4-chlorophenyl)thio]-1
(mothylamina) propyllabonyl actor monchydaeth (AGT)

(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX

NAME)

● HCl

RN 444645-51-6 CAPLUS

CN Carbamic acid, dimethyl-, 4-[3-[(4-fluorophenyl)thio]-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 444645-54-9 CAPLUS

CN Carbamic acid, dimethyl-, 4-[3-[(6-chloro-2-pyridinyl)oxy]-1- (methylamino)propyl]phenyl ester, dihydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{NHMe} \\ \text{O} \\ \text{Me}_2 \text{N} - \begin{array}{c} \text{C} \\ \text{H} \end{array} - \begin{array}{c} \text{C} \\ \text{C} \end{array} - \begin{array}{c} \text{C} \\$$

●2 HC1

RN 444645-56-1 CAPLUS
CN Carbamic acid, dimethyl-, 4-[(1S)-3-(3,4-difluorophenoxy)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX

NAME)

Absolute stereochemistry.

● HCl

RN 444645-62-9 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(methylamino)-3-[(6-nitro-2-pyridinyl)oxy]propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 444645-64-1 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(methylamino)-3-[[6-(trifluoromethyl)-2-

pyridinyl]oxy]propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 444645-66-3 CAPLUS

CN 2-Thiophenecarboxylic acid, 3-[3-[4-

[[(dimethylamino)carbonyl]oxy]phenyl]3-(methylamino)propoxy]-, methyl ester (9CI) (CA INDEX NAME)

RN 444645-69-6 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(methylamino)-3-[4-(methylthio)phenoxy]propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HC1

RN 444645-73-2 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(methylamino)-3-(pentafluorophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 444645-78-7 CAPLUS

CN Carbamic acid, dimethyl-, 2-methyl-4-[(1S)-1-(methylamino)-3-(4-nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX

NAME)

Absolute stereochemistry.

```
444643-93-0P 444644-00-2P 444644-01-3P
IT
     444644-02-4P 444644-04-6P 444644-05-7P
     444644-06-8P 444644-08-0P 444644-09-1P
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     444646-62-2P 444667-95-2P 444667-97-4P
     444667-98-5P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of alkylcarbamic acid esters as acetylcholinesterase
inhibitor)
     444643-93-0 CAPLUS
    Carbamic acid, dimethyl-, 3-[1-(dimethylamino)-3-(4-
```

$$\begin{array}{c} \text{O} \\ \text{Me 2N-C-O} \end{array} \begin{array}{c} \text{NMe 2} \\ \text{CH-CH}_2\text{-CH}_2 \end{array} \begin{array}{c} \text{OMe} \\ \end{array}$$

CN

NAME)

HC1

RN 444644-00-2 CAPLUS Carbamic acid, dimethyl-, 3-[1-(methylamino)-3-[4-CN (trifluoromethyl)phenyl]propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

methoxyphenyl)propyl]phenyl ester, monohydrochloride (9CI)

(CA INDEX

$$\begin{array}{c} \text{O} \\ \text{Me} \, 2\text{N} - \text{C} - \text{O} \end{array} \begin{array}{c} \text{NHMe} \\ \text{CH} - \text{CH}_2 - \text{CH}_2 \end{array} \begin{array}{c} \text{CF3} \\ \end{array}$$

HC1

RN444644-01-3 CAPLUS Carbamic acid, dimethyl-, 3-[3-(3,4-dimethoxyphenyl)-1-(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{OMe} \\ \text{NHMe} \\ \text{Me}_2\text{N} - \begin{array}{c} \text{O} \\ \text{CH} - \text{CH}_2 - \text{CH}_2 \end{array} \end{array} \begin{array}{c} \text{OMe} \\ \text{OMe}$$

● HCl

RN 444644-02-4 CAPLUS

CN Carbamic acid, dimethyl-, 3-[3-(1,3-benzodioxol-5-yl)-1- (methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 444644-04-6 CAPLUS

INDEX NAME)

HC1

RN 444644-05-7 CAPLUS

CN Carbamic acid, dimethyl-, 3-[3-(4-methoxyphenoxy)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HCl

RN 444644-06-8 CAPLUS

CN Carbamic acid, dimethyl-, 3-[1-(methylamino)-3-(4-methylphenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{NHMe} \\ \text{Me}_2\text{N} - \begin{array}{c} \text{C}_{-0} \\ \text{CH} - \text{CH}_2 - \text{CH}_2 - \text{O} \end{array} \end{array}$$

HC1

RN 444644-08-0 CAPLUS
CN Carbamic acid, dimethyl-, 3-[3-(4-fluorophenoxy)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$0 \qquad \qquad \begin{array}{c} NHMe \\ CH-CH_2-CH_2-O \end{array}$$

HC1

RN 444644-09-1 CAPLUS
CN Carbamic acid, ethyl-, 3-[3-(4-fluorophenoxy)-1-(methylamino)propyl]phenyl
ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

● HCl

RN 444644-11-5 CAPLUS
CN Propanoic acid, 2,2-dimethyl-, 3-[3-(4-fluorophenoxy)-1(methylamino)propyl]phenyl ester, hydrochloride (9CI) (CA INDEX NAME)

HC1

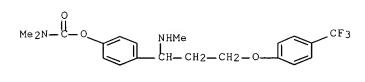
$$\begin{array}{c} \text{NHMe} \\ \text{Me}_2\text{N} - \begin{array}{c} \text{C} \\ \text{O} \end{array} \end{array}$$

HCl

RN 444644-13-7 CAPLUS
CN Carbamic acid, dimethyl-, 4-[3-(4-chlorophenoxy)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HCl

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HC1

RN 444644-15-9 CAPLUS

CN Carbamic acid, dimethyl-, 4-[3-(4-methoxyphenoxy)-1-(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 444644-16-0 CAPLUS

CN Carbamic acid, dimethyl-, 3-[1-amino-3-(4-fluorophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 444644-17-1 CAPLUS

CN Carbamic acid, dimethyl-, 3-[1-(ethylamino)-3-(4-fluorophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HCl

RN 444644-18-2 CAPLUS

CN Carbamic acid, dimethyl-, 3-[3-(4-fluorophenoxy)-1-(propylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HC1

RN 444644-19-3 CAPLUS

CN Carbamic acid, dimethyl-, 3-[4-(4-fluorophenyl)-1(methylamino)butyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HC1

RN 444644-20-6 CAPLUS

CN Carbamic acid, diethyl-, 3-[3-(4-fluorophenoxy)-1- (methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \mathsf{O} & \mathsf{N}\,\mathsf{HMe} \\ \mathsf{Et}\,\mathsf{2N}-\mathsf{C}-\mathsf{O} & \mathsf{CH}_2-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{O} \end{array}$$

HC1

RN 444644-21-7 CAPLUS

HCl

RN 444644-22-8 CAPLUS

CN 4-Morpholinecarboxylic acid, 3-[3-(4-fluorophenoxy)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

$$\begin{array}{c} \text{NMe 2} \\ \text{Me 2N-CH_2-CH_2-O} \end{array}$$

HC1

RN 444644-24-0 CAPLUS
CN Carbamic acid, dimethyl-, 3-[1-(dimethylamino)-3-(4-fluorophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

$$\begin{array}{c} \text{Me 2N-C-O} \\ \text{Me 2N-CH_2-O} \\ \text{CH-CH_2-CH_2-O} \end{array}$$

HC1

RN 444644-27-3 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(dimethylamino)-3-(4-fluorophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me}_{2}\text{N} - \overset{\text{O}}{\text{C}} + \text{O} \\ & \text{CH} - \text{CH}_{2} - \text{CH}_{2} - \text{O} \end{array}$$

● HCl

RN 444644-28-4 CAPLUS

CN Carbamic acid, dimethyl-, 3-[3-(4-fluorophenyl)-1-(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 444644-29-5 CAPLUS

CN Carbamic acid, dimethyl-, 4-[3-(4-fluorophenyl)-1- (methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ Me\ 2N - C - O \\ \hline \\ CH - CH2 - CH2 \end{array}$$

● HCl

RN 444644-30-8 CAPLUS

CN Carbamic acid, dimethyl-, 3-[4-(4-chlorophenyl)-1- (methylamino)butyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HC1

● HCl

RN 444644-32-0 CAPLUS
CN Carbamic acid, dimethyl-, 4-[3-(3-methoxyphenoxy)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$Me_2N = \bigcup_{CH = CH_2 - CH_2 - O}^{OHMe} OMe$$

● HCl

RN 444644-33-1 CAPLUS
CN Carbamic acid, dimethyl-, 4-[3-(2-methoxyphenoxy)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

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● HCl

RN 444644-34-2 CAPLUS

CN Carbamic acid, dimethyl-, 4-[3-(3-chlorophenoxy)-1- (methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me}_2\text{N} - \overset{\text{O}}{\text{C}} - \text{O} \\ & \text{CH} - \text{CH}_2 - \text{CH}_2 - \text{O} \\ & \text{C1} \end{array}$$

HC1

RN 444644-35-3 CAPLUS

CN Carbamic acid, dimethyl-, 4-[3-(2-chlorophenoxy)-1- (methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 444644-36-4 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(methylamino)-3-(4-methylphenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 444644-37-5 CAPLUS

CN Carbamic acid, dimethyl-, 4-[3-(4-chlorophenoxy)-1(dimethylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HC1

RN 444644-38-6 CAPLUS

CN Carbamic acid, dimethyl-, 4-[3-(4-chlorophenyl)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me}\, 2\text{N} - \overset{\text{O}}{\text{C}} - \text{O} \\ & \text{CH} - \text{CH}_2 - \text{CH}_2 \end{array} \end{array}$$

● HCl

RN 444644-39-7 CAPLUS
CN Carbamic acid, dimethyl-, 4-[3-(2,4-difluorophenoxy)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me}_2\text{N} - \overset{\text{O}}{\text{C}} = 0 \\ \text{O} & \text{NHMe} \\ \text{CH-CH}_2 - \text{CH}_2 - \text{O} \\ \text{F} \end{array}$$

● HCl

RN 444644-40-0 CAPLUS

CN Carbamic acid, dimethyl-, 4-[3-(2-chloro-4-fluorophenoxy)-1- (methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HC1

RN 444644-41-1 CAPLUS
CN Carbamic acid, dimethyl-, 4-[3-(4-acetylphenoxy)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 444644-42-2 CAPLUS
CN Carbamic acid, dimethyl-, 4-[3-(2,4-dichlorophenoxy)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 444644-43-3 CAPLUS
CN Carbamic acid, dimethyl-, 4-[3-(3,4-dichlorophenoxy)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 444644-44 CAPLUS
CN Carbamic acid, dimethyl-, 4-[1-(methylamino)-3-(4nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX
NAME)

HC1

RN 444644-45-5 CAPLUS
CN Carbamic acid, dimethyl-, 4-[3-(4-aminophenoxy)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HC1

RN 444644-46-6 CAPLUS
CN Carbamic acid, dimethyl-, 4-[3-[4-(acetylamino)phenoxy]-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HC1

RN 444644-47-7 CAPLUS
CN Carbamic acid, dimethyl-, 4-[3-(3-chlorophenoxy)-1(dimethylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

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$$\begin{array}{c} \text{Me}\,2\text{N} - \overset{\text{O}}{\text{C}} - \text{O} & \text{NMe}\,2 \\ \text{CH-CH}_2 - \text{CH}_2 - \text{O} & \text{C1} \end{array}$$

RN 444644-48-8 CAPLUS

CN Carbamic acid, dimethyl-, 4-[3-(2-chlorophenoxy)-1-(dimethylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me 2N-C-O} \\ \text{Me 2N-CH_2-CH_2-O} \end{array}$$

● HCl

RN 444644-49-9 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(methylamino)-3-(3-nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me}_{\,2}\text{N} - \overset{\text{O}}{\text{C}} - \text{O} & \text{NHMe} \\ \text{CH}_{\,2}\text{CH}_{\,2} - \text{CH}_{\,2} - \text{O} & \text{NO}_{\,2} \end{array}$$

HCl

RN 444644-50-2 CAPLUS

CN Carbamic acid, dimethyl-, 4-[3-(3,4-difluorophenoxy)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 444644-51-3 CAPLUS

CN Carbamic acid, dimethyl-, 4-[3-(4-chloro-3-fluorophenoxy)-1-(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HC1

RN 444644-52-4 CAPLUS

CN Carbamic acid, dimethyl-, 4-[3-(4-cyanophenoxy)-1- (methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 444644-53-5 CAPLUS

CN Carbamic acid, dimethyl-, 4-[3-(4-bromophenoxy)-1- (methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 444644-54-6 CAPLUS

CN Carbamic acid, dimethyl-, 4-[3-(4-fluoro-2-methylphenoxy)-1- (methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HCl

RN 444644-55-7 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(methylamino)-3-(3-methylphenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HC1

RN 444644-56-8 CAPLUS CN Carbamic acid, dimethyl-, 4-[3-(3,4-dimethylphenoxy)-1-

(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \ 2\text{N} - \text{C} - \text{O} \\ \text{NHMe} \\ \text{CH-CH} \ 2 - \text{CH} \ 2 - \text{O} \\ \end{array}$$

HC1

RN 444644-57-9 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1R)-3-(3-chlorophenoxy)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 444644-58-0 CAPLUS
CN Carbamic acid, dimethyl-, 4-[(1R)-3-(4-chlorophenoxy)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX

Absolute stereochemistry.

NAME)

● HCl

RN 444644-60-4 CAPLUS
CN Carbamic acid, dimethyl-, 4-[3-(3-aminophenoxy)-1(methylamino)propyl]phenyl ester, dihydrochloride (9CI) (CA INDEX
NAME)

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$$\begin{array}{c} \text{Me}\,_2\text{N} \\ \begin{array}{c} \text{C} \\ \end{array} \\ \begin{array}{c} \text{C} \\ \end{array} \\ \begin{array}{c} \text{N}\,_2\text{MMe} \\ \\ \text{C}\,_1\text{C}\,_2\text{C}\,_2\text{C}\,_2\text{C} \\ \end{array} \\ \begin{array}{c} \text{N}\,_1\text{M}\,_2\text{C} \\ \end{array}$$

●2 HC1

RN 444644-61-5 CAPLUS

CN Carbamic acid, dimethyl-, 4-[3-[3-(acetylamino)phenoxy]-1- (methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me}\, 2\text{N} - \overset{\text{O}}{\text{C}} - \text{O} \\ \\ \text{CH} - \text{CH}_2 - \text{CH}_2 - \text{O} \\ \\ \end{array} \\ \begin{array}{c} \text{NHAc} \\ \\ \text{NHAc} \end{array}$$

● HCl

RN 444644-62-6 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(methylamino)-3-(2-nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HCl

RN 444644-63-7 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(methylamino)-3-phenoxypropyl] phenyl ester,

monohydrochloride (9CI) (CA INDEX NAME)

HCl

RN 444644-64-8 CAPLUS

CN Carbamic acid, dimethyl-, 4-[3-(3-fluorophenoxy)-1-(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me}_{2}\text{N} - \overset{\text{O}}{\text{C}} - \text{O} \\ & \text{CH-CH}_{2} - \text{CH}_{2} - \text{O} \\ & \text{F} \end{array}$$

HC1

RN 444644-65-9 CAPLUS

CN Carbamic acid, dimethyl-, 4-[3-(2-fluorophenoxy)-1- (methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me}\,2\text{N} - \overset{\text{O}}{\text{C}} - \text{O} \\ & \text{NHMe} \end{array} \qquad \begin{array}{c} \text{F} \\ \text{CH-CH2-CH2-O} \end{array}$$

● HCl

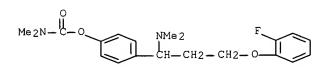
RN 444644-66-0 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(dimethylamino)-3-(3-fluorophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 444644-67-1 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(dimethylamino)-3-(2-fluorophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)



HC1

RN 444644-68-2 CAPLUS
CN Carbamic acid, dimethyl-, 4-[3-(3-acetylphenoxy)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me}\, 2\text{N} - \overset{\text{O}}{\text{C}} - \text{O} \\ \\ \text{CH-} \, \text{CH}_2 - \text{CH}_2 - \text{O} \\ \\ \end{array}$$

● HCl

RN 444644-69-3 CAPLUS
CN Carbamic acid, dimethyl-, 4-[3-(4-chloro-3-methylphenoxy)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 444644-70-6 CAPLUS
CN Carbamic acid, dimethyl-, 4-[3-(3-chloro-4-fluorophenoxy)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HCl

RN 444644-71-7 CAPLUS

CN Carbamic acid, dimethyl-, 4-[3-(4-acetylphenoxy)-1-(dimethylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HC1

RN 444644-72-8 CAPLUS

CN Carbamic acid, dimethyl-, 4-[3-(3,4-difluorophenoxy)-1-(dimethylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me}\, 2\text{N} - \overset{\text{O}}{\text{C}} - \text{O} \\ & \text{NMe}\, 2 \\ \text{CH} - \text{CH}\, 2 - \text{CH}\, 2 - \text{O} \\ \end{array}$$

● HCl

RN 444644-73-9 CAPLUS

CN Carbamic acid, diethyl-, 4-[3-(3-chlorophenoxy)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Et2N-CONTRACTORS} \\ \text{CH-CH2-CH2-ONTRACTORS} \\ \text{C1} \end{array}$$

HCl

RN 444644-74-0 CAPLUS

CN Carbamic acid, dimethyl-, 4-[3-(4-chloro-3-fluorophenoxy)-1-(dimethylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$Me_2N = C - O \qquad NMe_2$$

$$CH = CH_2 - CH_2 - O \qquad F$$

RN 444644-75-1 CAPLUS

CN Carbamic acid, dimethyl-, 4-[3-(3,5-difluorophenoxy)-1- (methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 444644-77-3 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1S)-3-(3-chlorophenoxy)-1- (methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 444644-79-5 CAPLUS

CN Carbamic acid, ethylmethyl-, 4-[3-(4-chlorophenoxy)-1-(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HC1

RN 444644-80-8 CAPLUS

CN Carbamic acid, dimethyl-, 4-[3-(3,5-difluorophenoxy)-1-(dimethylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me}_2\text{N} - \overset{\circ}{\text{C}} - \text{O} \\ & \text{CH} - \text{CH}_2 - \text{CH}_2 - \text{O} \\ & \text{F} \end{array}$$

● HCl

RN 444644-81-9 CAPLUS

CN Carbamic acid, dimethyl-, 4-[3-(2,4-difluorophenoxy)-1-(dimethylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 444644-82-0 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(dimethylamino)-3-(3nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me}_2\text{N} \\ -\text{C} \\ -\text{C} \\ -\text{CH}_2\text{CH}_2\text{-CH}_2\text{-O} \\ -\text{NO}_2 \\ \end{array}$$

● HCl

RN 444644-83-1 CAPLUS

CN Carbamic acid, dimethyl-, 4-[3-[(3-chlorophenyl)amino]-1- (methylamino)propyl]phenyl ester, dihydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me}\,2\text{N} - \overset{\text{O}}{\text{C}} - \text{O} \\ \text{CH} - \text{CH}_2 - \text{CH}_2 - \text{NH} \end{array}$$

RN 444644-84-2 CAPLUS
CN Carbamic acid, dimethyl-, 4-[3-(3-fluoro-4-nitrophenoxy)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me}_{2}\text{N} - \overset{\text{O}}{\text{C}} - \text{O} & \overset{\text{N}_{1}\text{MMe}}{\text{CH} - \text{CH}_{2} - \text{CH}_{2} - \text{O}} & \overset{\text{F}}{\text{N}} & \text{NO}_{2} \\ \end{array}$$

HCl

● HCl

RN 44464-86-4 CAPLUS
CN Carbamic acid, dimethyl-, 4-[3-(4-chloro-3-nitrophenoxy)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HC1

RN 444644-87-5 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(methylamino)-3-(2,3,5-trifluorophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX

NAME)

HC1

RN 444644-88-6 CAPLUS
CN Carbamic acid, dimethyl-, 4-[3-[(3-fluorophenyl)amino]-1(methylamino)propyl]phenyl ester, dihydrochloride (9CI) (CA INDEX NAME)

●2 HC1

RN 444644-89-7 CAPLUS
CN Carbamic acid, dimethyl-, 3-[3-(3-fluorophenoxy)-1-

(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HC1

RN 444644-90-0 CAPLUS

CN Carbamic acid, dimethyl-, 3-[1-(methylamino)-3-(4-nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

RN 444644-91-1 CAPLUS
CN Carbamic acid, dimethyl-, 4-[3-(2-fluoro-4-nitrophenoxy)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

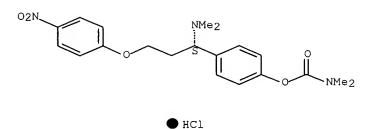
● HCl

RN 444644-92-2 CAPLUS
CN Carbamic acid, dimethyl-, 4-[3-[(4-fluorophenyl)amino]-1(methylamino)propyl]phenyl ester, dihydrochloride (9CI) (CA INDEX NAME)

●2 HC1

RN 444644-94-4 CAPLUS
CN Carbamic acid, dimethyl-, 4-[(1S)-1-(dimethylamino)-3-(4-nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 444644-95-5 CAPLUS
CN Carbamic acid, dimethyl-, 4-[(1R)-1-amino-3-(4-nitrophenoxy)propyl]phenyl
ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

HC1

RN 444644-96-6 CAPLUS
CN Carbamic acid, dimethyl-, 4-[(1R)-1-(methylamino)-3-(4-nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 444644-97-7 CAPLUS
CN Carbamic acid, dimethyl-, 4-[(1R)-1-(dimethylamino)-3-(4-nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\underbrace{ \begin{array}{c} \text{MeNH} \\ \text{O-CH}_2\text{-CH}_2\text{-CH} \end{array} } \underbrace{ \begin{array}{c} \text{O-} \\ \text{C-NMe} \ 2 \end{array}$$

●2 HC1

RN 444644-99-9 CAPLUS
CN Carbamic acid, dimethyl-, 3-[1-(dimethylamino)-3-(4-nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 444645-00-5 CAPLUS
CN Carbamic acid, dimethyl-, 4-[1-(ethylamino)-3-(3-nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 444645-01-6 CAPLUS
CN Carbamic acid, dimethyl-, 4-[1-(ethylamino)-3-(4-fluorophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HC1

RN 444645-02-7 CAPLUS
CN Carbamic acid, dimethyl-, 4-[1-(ethylamino)-3-(3-fluorophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 444645-03-8 CAPLUS
CN Carbamic acid, dimethyl-, 3-[1-(methylamino)-3-(3nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX
NAME)

● HCl

RN 444645-04-9 CAPLUS
CN Carbamic acid, dimethyl-, 4-[3-[(4-chlorophenyl)amino]-1(methylamino)propyl]phenyl ester, dihydrochloride (9CI) (CA INDEX NAME)

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$$Me_2N = COO_{COO_{CH-CH_2-CH_2-NH-COO_{COO_{CH-CH_2-NH-COO_{COO_{COO_{CH-COO$$

RN 444645-05-0 CAPLUS

CN Carbamic acid, dimethyl-, 4-[3-[acetyl(3-fluorophenyl)amino]-1- (methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 444645-06-1 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(methylamino)-3-(3-methyl-4-nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 444645-07-2 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(methylamino)-3-(2-methylphenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 444645-08-3 CAPLUS
CN Carbamic acid, dimethyl-, 4-[3-(4-chloro-2-methylphenoxy)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HCl

RN 444645-09-4 CAPLUS
CN Carbamic acid, dimethyl-, 4-[1-(dimethylamino)-3-(3,4,5-trifluorophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 444645-10-7 CAPLUS
CN Carbamic acid, dimethyl-, 4-[4-(4-chlorophenoxy)-1(methylamino)butyl]phenyl ester, monohydrochloride (9CI) (CA INDEX
NAME)

HCl

RN 444645-11-8 CAPLUS
CN Carbamic acid, dimethyl-, 4-[1-(methylamino)-4-(4nitrophenoxy)butyl]phenyl ester, monohydrochloride (9CI) (CA INDEX
NAME)

RN 444645-12-9 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(methylamino)-2-(4-nitrophenoxy)ethyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me}\, 2\text{N} - \overset{\text{O}}{\text{C}} - \text{O} \\ \\ \text{CH} - \text{CH}\, 2 - \text{O} \\ \end{array}$$

HC1

RN 444645-13-0 CAPLUS

CN Carbamic acid, dimethyl-, 4-[3-[acetyl(4-chlorophenyl)amino]-1- (methylamino)propyl]phenyl ester, dihydrochloride (9CI) (CA INDEX NAME)

●2 HC1

RN 444645-14-1 CAPLUS

CN Carbamic acid, dimethyl-, 4-[3-[acetyl(4-nitrophenyl)amino]-1- (methylamino)propyl]phenyl ester, dihydrochloride (9CI) (CA INDEX NAME)

●2 HCl

●2 HC1

Me
$$_2$$
N $_{-}$ C $_{-}$ O $_{-}$ NHMe $_{-}$ CH $_{-}$ CH $_{2}$ CH $_{2}$ CH $_{2}$

RN 444645-17-4 CAPLUS
CN Carbamic acid, dimethyl-, 4-[(1S)-1-amino-3-(4-nitrophenoxy)propyl]phenyl
ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 444645-19-6 CAPLUS
CN Carbamic acid, dimethyl-, 3-[(1S)-1-(methylamino)-3-(4nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX
NAME)

Absolute stereochemistry.

RN 444645-20-9 CAPLUS
CN Carbamic acid, dimethyl-, 3-[(1s)-1-(dimethylamino)-3-(4-nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 444645-21-0 CAPLUS
CN Carbamic acid, dimethyl-, 3-[(1S)-3-(2-chloro-4-nitrophenoxy)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

HC1

RN 444645-23-2 CAPLUS
CN Carbamic acid, dimethyl-, 3-[(1S)-3-(2-chloro-4-nitrophenoxy)-1(dimethylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 444645-24-3 CAPLUS

CN Carbamic acid, dimethyl-, 3-[(1R)-3-(2-chloro-4-nitrophenoxy)-1-(dimethylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 444645-25-4 CAPLUS

CN Carbamic acid, dimethyl-, 3-[3-(2-chloro-4-nitrophenoxý)-1-(dimethylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{NMe 2} \\ \text{Me 2N-CH2-CH2-O} \end{array}$$

HC1

RN 444645-26-5 CAPLUS

CN Carbamic acid, dimethyl-, 3-[3-[(5-chloro-3-pyridinyl)oxy]-1- (methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

RN 444645-27-6 CAPLUS

CN Carbamic acid, dimethyl-, 3-[1-(methylamino)-3-[(6-methyl-3-pyridinyl)oxy]propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me}\,2\text{N} - \overset{\text{O}}{\text{C}} - \text{O} \\ \end{array} \begin{array}{c} \text{N}\,\text{HMe} \\ \text{CH}-\,\text{CH}_2-\,\text{CH}_2-\,\text{O} \\ \end{array} \begin{array}{c} \text{N} \\ \text{Me} \end{array}$$

HC1

RN 444645-28-7 CAPLUS

CN Carbamic acid, dimethyl-, 3-[1-(methylamino)-3-[(2-methyl-3-pyridinyl)oxy]propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ Me \\ 2N - C - O \end{array}$$

$$\begin{array}{c} N \\ HMe \\ CH - CH_2 - CH_2 - O \end{array}$$

● HCl

RN 444645-30-1 CAPLUS

CN Carbamic acid, dimethyl-, 3-[(1R)-1-(dimethylamino)-3-(4-nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 444645-32-3 CAPLUS
CN Carbamic acid, dimethyl-, 4-[1-(ethylmethylamino)-3-(4nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX
NAME)

$$\begin{array}{c} \text{Me}_{2N} - \overset{\text{O}}{\text{C}} - \overset{\text{Me}}{\text{O}} & \overset{\text{Me}}{\text{N-Et}} \\ \text{N-Et} & \overset{\text{NO}_{2}}{\text{CH-CH}_{2}-\text{CH}_{2}-\text{O}} \end{array}$$

● HCl

HC1

RN 444645-36-7 CAPLUS
CN Carbamic acid, dimethyl-, 4-[3-(3,4-difluorophenoxy)-1(ethylmethylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA
INDEX
NAME)

● HCl

NAME)

RN 444645-39-0 CAPLUS
CN Carbamic acid, dimethyl-, 3-[3-(4-chlorophenoxy)-1(dimethylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX

HC1

RN 444645-42-5 CAPLUS
CN Carbamic acid, dimethyl-, 3-[3-(3-chlorophenoxy)-1(dimethylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{O} \\ \text{Me} \, 2\text{N} - \text{C} - \text{O} \end{array} \begin{array}{c} \text{NMe} \, 2 \\ \text{CH} - \text{CH}_2 - \text{CH}_2 - \text{O} \end{array} \begin{array}{c} \text{C1} \\ \text{C1} \end{array}$$

● HCl

RN 444645-43-6 CAPLUS
CN Carbamic acid, dimethyl-, 3-[3-(3-chloro-4-fluorophenoxy)-1(dimethylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

RN 444645-44-7 CAPLUS

CN Carbamic acid, dimethyl-, 3-[3-(4-chloro-3-fluorophenoxy)-1-(dimethylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 444645-46-9 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1R)-3-(3,4-difluorophenoxy)-1-(dimethylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 444645-48-1 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(dimethylamino)-3-[(4-nitrophenyl)thio]propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX

NAME)

RN 444645-50-5 CAPLUS
CN Carbamic acid, dimethyl-, 4-[3

CN Carbamic acid, dimethyl-, 4-[3-[(4-chlorophenyl)thio]-1-(dimethylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HC1

RN 444645-52-7 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(dimethylamino)-3-[(4-fluorophenyl)thio]propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX

NAME)

HCl

RN 444645-53-8 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(dimethylamino)-3-(2-pyridinyloxy)propyl]phenyl ester, dihydrochloride (9CI) (CA INDEX NAME)

●2 HCl

RN 444645-55-0 CAPLUS
CN Carbamic acid, dimethyl-, 4-[3-[(6-chloro-2-pyridinyl)oxy]-1(dimethylamino)propyl]phenyl ester, dihydrochloride (9CI) (CA INDEX NAME)

●2 HCl

RN 444645-57-2 CAPLUS
CN Carbamic acid, dimethyl-, 4-[(1S)-3-(3,4-difluorophenoxy)-1(dimethylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

HCl

RN 444645-59-4 CAPLUS
CN Carbamic acid, dimethyl-, 4-[(1S)-3-(4-chlorophenoxy)-1(methylamino)propyl]phenyl ester, (2E)-2-butenedioate (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 444645-58-3 CMF C19 H23 C1 N2 O3

Absolute stereochemistry.

CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

RN 444645-60-7 CAPLUS

CN Benzoic acid, 4-[3-[4-[[(dimethylamino)carbonyl]oxy]phenyl]-3-(methylamino)propoxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me}_{2}\text{N} - \overset{\circ}{\text{U}} - \overset{\circ}{\text{U}} - \overset{\circ}{\text{U}} - \overset{\circ}{\text{U}} + \overset{\circ}{\text{U}} + \overset{\circ}{\text{U}} - \overset{\circ}{\text{U}} + \overset{\circ}{\text{U}} - \overset{\circ}{\text{U$$

RN 444645-61-8 CAPLUS

CN Benzoic acid, 4-[3-(dimethylamino)-3-[4-[(dimethylamino)carbonyl]oxy]phen

yl]propoxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me}_{2}\text{N} = \overset{\circ}{\text{C}} = 0 \\ \text{CH} = \text{CH}_{2} = \text{CH}_{2} = 0 \end{array}$$

RN 444645-63-0 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(dimethylamino)-3-[(6-nitro-2-pyridinyl)oxy]propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HC1

RN 444645-65-2 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(dimethylamino)-3-[[6-(trifluoromethyl)-2-

pyridinyl]oxy]propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{NMe}_2 \\ \text{CH-CH}_2\text{-CH}_2\text{-CH}_2\text{-O} \\ \text{CF}_3 \end{array}$$

HCl

RN 444645-67-4 CAPLUS
CN 2-Thiophenecarboxylic acid, 3-[3-(dimethylamino)-3-[4 [[(dimethylamino)carbonyl]oxy]phenyl]propoxy]-, methyl ester (9CI)
(CA
 INDEX NAME)

$$\begin{array}{c} \text{Me}_{\,2}\text{N} - \overset{\text{\scriptsize 0}}{\text{\scriptsize C}} - \text{\scriptsize 0} & \text{\scriptsize NHMe} \\ \text{\scriptsize CH}_{\,2} - \text{\scriptsize CH}_{\,2} - \text{\scriptsize CH}_{\,2} - \text{\scriptsize 0} & \text{\scriptsize NO}_{\,2} \end{array}$$

● HCl

RN 444645-70-9 CAPLUS
CN Carbamic acid, dimethyl-, 4-[1-(dimethylamino)-3-[4-

(methylthio)phenoxy]propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 444645-71-0 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1S)-1-(methylamino)-3-[4-(methylthio)phenoxy]propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 444645-72-1 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1R)-1-(methylamino)-3-[4-(methylthio)phenoxy]propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

HCl

RN 444645-75-4 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-(methylamino)-3-(6-quinolinyloxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HC1

RN 444645-76-5 CAPLUS

● HCl

RN 444645-77-6 CAPLUS
CN Carbamic acid, dimethyl-, 4-[1-(dimethylamino)-3-(4-nitrophenoxy)propyl]-3methylphenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HC1

RN 444645-79-8 CAPLUS
CN Carbamic acid, dimethyl-, 2-methyl-4-[(1R)-1-(methylamino)-3-(4-nitrophenoxy)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

HCl

RN 444645-80-1 CAPLUS
CN Carbamic acid, dimethyl-, 4-[3-(4-chlorophenoxy)-1-(dimethylamino)propyl]2-methylphenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

● HCl

RN 444645-83-4 CAPLUS
CN Carbamic acid, dimethyl-, 1-[2-(4-chloro-3-methylphenoxy)ethyl]1,2,3,4tetrahydro-2-methyl-6-isoquinolinyl ester, monohydrochloride (9CI)
(CA
INDEX NAME)

HCl

RN 444645-84-5 CAPLUS
CN Carbamic acid, dimethyl-, 1-[2-(2-chloro-4-nitrophenoxy)ethyl]1,2,3,4tetrahydro-2-methyl-6-isoquinolinyl ester, monohydrochloride (9CI)
(CA
INDEX NAME)

$$C1$$
 $C1$
 CH_2
 CH_2

● HCl

RN 444645-85-6 CAPLUS
CN Carbamic acid, dimethyl-, (1R)-1-[2-(2-chloro-4-nitrophenoxy)ethyl]1,2,3,4-tetrahydro-2-methyl-6-isoquinolinyl ester, monohydrochloride
(9CI)
(CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 444645-86-7 CAPLUS
CN Carbamic acid, dimethyl-, 1-[2-(4-chlorophenoxy)ethyl]-1,2,3,4tetrahydro2-methyl-7-isoquinolinyl ester, monohydrochloride (9CI) (CA INDEX
NAME)

$$\begin{array}{c} C1 \\ CH_2 \\ CH_2 \\ CH_2 \\ \end{array}$$

$$\begin{array}{c} Me_2N - \\ Me_2N - \\ \end{array}$$

$$\begin{array}{c} O \\ Me_2N - \\ \end{array}$$

$$\begin{array}{c} O \\ N \\ \end{array}$$

RN 444645-88-9 CAPLUS
CN Carbamic acid, dimethyl-, 1-[2-(2-chloro-4-nitrophenoxy)ethyl]2,3,4,5tetrahydro-2-methyl-1H-2-benzazepin-7-yl ester, monohydrochloride
(9CI)
(CA INDEX NAME)

444645-89-0 CAPLUS

Carbamic acid, dimethyl-, 1-[2-(4-chloro-3-methylphenoxy)ethyl]-2,3dihydro-2-methyl-1H-2-benzazepin-7-yl ester, monohydrochloride (9CI) (CA

INDEX NAME)

444645-90-3 CAPLUS RN

Carbamic acid, dimethyl-, 1-[2-(2-chloro-4-fluorophenoxy)ethyl]-2,3-CNdihydro-2-methyl-1H-2-benzazepin-7-yl ester, monohydrochloride (9CI)

(CA INDEX NAME)

RN 444645-91-4 CAPLUS
CN Carbamic acid, dimethyl-, 2,3-dihydro-2-methyl-1-[2-[4-(methylthio)phenoxy]ethyl]-1H-2-benzazepin-7-yl ester, monohydrochloride
(9CI) (CA INDEX NAME)

RN 444645-92-5 CAPLUS
CN Carbamic acid, dimethyl-, (1R)-2,3-dihydro-2-methyl-1-[2-[4-(methylthio)phenoxy]ethyl]-1H-2-benzazepin-7-yl ester,
monohydrochloride
(9CI) (CA INDEX NAME)

RN 444645-93-6 CAPLUS
CN Carbamic acid, dimethyl-, (1s)-2,3-dihydro-2-methyl-1-[2-[4-(methylthio)phenoxy]ethyl]-1H-2-benzazepin-7-yl ester,
monohydrochloride
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 444645-94-7 CAPLUS
CN Carbamic acid, dimethyl-, (1S)-2,3-dihydro-2-methyl-1-[2-(4-nitrophenoxy)ethyl]-1H-2-benzazepin-7-yl ester, monohydrochloride
(9CI)
(CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 444645-95-8 CAPLUS
CN Carbamic acid, dimethyl-, 1-[2-(4-chloro-3-methylphenoxy)ethyl]-2,3dihydro-2-methyl-1H-2-benzazepin-8-yl ester, monohydrochloride (9CI)
(CA
INDEX NAME)

RN 444645-96-9 CAPLUS
CN Carbamic acid, dimethyl-, 1-[2-(4-chloro-3-methylphenoxy)ethyl]-2,3dihydro-2-methyl-1H-2-benzazepin-6-yl ester, monohydrochloride (9CI)
(CA
INDEX NAME)

RN 444645-97-0 CAPLUS
CN Carbamic acid, dimethyl-, 3-[3-(4-chloro-3-nitrophenoxy)-1(methylamino)propyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 444646-62-2 CAPLUS

CN Carbamic acid, dimethyl-, (1R)-1-[2-(4-chloro-3-methylphenyl)ethyl]-1,2,3,4-tetrahydro-6-isoquinolinyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 444667-95-2 CAPLUS

CN Carbamic acid, dimethyl-, 4-[2-(4-chlorophenoxy)-1(methylamino)ethyl]phenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HC1

RN 444667-97-4 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1S)-1-(methylamino)-3-(4-nitrophenoxy)propyl]phenyl ester, (2E)-2-butenedioate (2:1) (9CI) (CA INDEX NAME)

CM 1

CRN 444667-96-3 CMF C19 H23 N3 O5

CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

RN 444667-98-5 CAPLUS

CN Carbamic acid, dimethyl-, (1R)-2,3-dihydro-2-methyl-1-[2-(4-nitrophenoxy)ethyl]-1H-2-benzazepin-7-yl ester, monohydrochloride (9CI)

(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

● HCl

444646-02-0P 444646-04-2P 444646-10-0P IΤ 444646-11-1P 444646-13-3P 444646-16-6P 444646-17-7P 444646-19-9P 444646-20-2P 444646-21-3P 444646-22-4P 444646-23-5P 444646-24-6P 444646-25-7P 444646-26-8P 444646-29-1P 444646-30-4P 444646-32-6P 444646-33-7P 444646-35-9P 444646-36-0P 444646-39-3P 444646-40-6P 444646-49-5P 444646-61-1P 444646-82-6P 444646-83-7P 444646-84-8P 444646-85-9P 444646-86-0P 444646-89-3P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of alkylcarbamic acid esters as acetylcholinesterase inhibitor) 444646-02-0 CAPLUS Carbamic acid, dimethyl-, 3-[1-[[(1,1dimethylethoxy) carbonyl]methylamino] -3-(4-methoxyphenyl)propyl]phenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me O} \\ \text{N-C-OBu-t} \\ \text{CH-CH}_2\text{-CH}_2 \end{array}$$

RN 444646-04-2 CAPLUS

CN Carbamic acid, [1-[3-[[(ethylamino)carbonyl]oxy]phenyl]-3-(4-methoxyphenyl)propyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \quad \text{O} \\ \text{N} \quad \text{C} \quad \text{OBu-t} \\ \text{CH} \quad \text{CH}_2 \quad \text{CH}_2 \end{array} \\ \text{OMe}$$

RN 444646-10-0 CAPLUS

CN Carbamic acid, dimethyl-, 3-[1-[[(1,1-

dimethylethoxy) carbonyl]methylamino] -

3-[4-(trifluoromethyl)phenoxy]propyl]phenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me O} \\ \text{N-C-OBu-t} \\ \text{CH-CH}_2\text{-CH}_2\text{-O} \end{array}$$

RN 444646-11-1 CAPLUS

CN Carbamic acid, dimethyl-, 3-[1-[[(1,1-

dimethylethoxy)carbonyl]methylamino]-

3-(4-fluorophenoxy)propyl]phenyl ester (9CI) (CA INDEX NAME)

RN 444646-13-3 CAPLUS

CN Carbamic acid, [1-[3-(acetyloxy)phenyl]-3-(4-

fluorophenoxy) propyl]methyl-,

1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 444646-16-6 CAPLUS

CN Carbamic acid, dimethyl-, 3-[1-[[(1,1-dimethylethoxy)carbonyl]amino]-3-(4-

fluorophenoxy)propyl]phenyl ester (9CI) (CA INDEX NAME)

RN 444646-17-7 CAPLUS

CN Carbamic acid, dimethyl-, 3-[1-[(1,1-

dimethylethoxy)carbonyl]ethylamino]-

3-(4-fluorophenoxy)propyl]phenyl ester (9CI) (CA INDEX NAME)

RN 444646-19-9 CAPLUS

CN Carbamic acid, dimethyl-, 3-[1-[[(1,1-

dimethylethoxy)carbonyl]methylamino]-

4-(4-fluorophenyl)-3-butenyl]phenyl ester (9CI) (CA INDEX NAME)

RN 444646-20-2 CAPLUS

CN Carbamic acid, dimethyl-, 3-[1-[[(1,1-

dimethylethoxy)carbonyl]methylamino]-

4-(4-fluorophenyl)butyl]phenyl ester (9CI) (CA INDEX NAME)

RN 444646-21-3 CAPLUS

CN Carbamic acid, diethyl-, 3-[1-[[(1,1-

dimethylethoxy)carbonyl]methylamino]-

3-(4-fluorophenoxy)propyl]phenyl ester (9CI) (CA INDEX NAME)

RN 444646-22-4 CAPLUS

CN Carbamic acid, [3-(3-chlorophenoxy)-1-[4-

[[(dimethylamino)carbonyl]oxy]phe

nyl]propyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 444646-23-5 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-[(1,1-

dimethylethoxy)carbonyl]methylamino]-

3-(4-nitrophenoxy)propyl]phenyl ester (9CI) (CA INDEX NAME)

RN 444646-24-6 CAPLUS

CN Carbamic acid, [3-(4-aminophenoxy)-1-[4-

[[(dimethylamino)carbonyl]oxy]phen

yl]propyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 444646-25-7 CAPLUS

CN Carbamic acid, [3-[4-(acetylamino)phenoxy]-1-[4-[[(dimethylamino)carbonyl]oxy]phenyl]propyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 444646-26-8 CAPLUS

CN Carbamic acid, dimethyl-, 4-[1-[(1,1-

dimethylethoxy)carbonyl]methylamino]-

3-(3-nitrophenoxy)propyl]phenyl ester (9CI) (CA INDEX NAME)

RN 444646-29-1 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1R)-3-(3-chlorophenoxy)-1-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 444646-30-4 CAPLUS

CN Carbamic acid, [(1R)-3-(3-chlorophenoxy)-1-[4-[[(dimethylamino)carbonyl]oxy]phenyl]propyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 444646-32-6 CAPLUS
CN Carbamic acid, [3-(3-aminophenoxy)-1-[4[[(dimethylamino)carbonyl]oxy]phen
 yl]propyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 444646-33-7 CAPLUS
CN Carbamic acid, [3-[3-(acetylamino)phenoxy]-1-[4[[(dimethylamino)carbonyl]oxy]phenyl]propyl]methyl-, 1,1-dimethylethyl
ester (9CI) (CA INDEX NAME)

RN 444646-35-9 CAPLUS
CN Carbamic acid, [3-(4-chlorophenoxy)-1-[4[[(ethylmethylamino)carbonyl]oxy]
 phenyl]propyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 444646-36-0 CAPLUS
CN Carbamic acid, [3-[(3-chlorophenyl)amino]-1-[4[[(dimethylamino)carbonyl]oxy]phenyl]propyl]methyl-, 1,1-dimethylethyl
ester (9CI) (CA INDEX NAME)

RN 444646-39-3 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1S)-1-[[(1,1-

dimethylethoxy)carbonyl]methyla

mino]-3-(4-nitrophenoxy)propyl]phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 444646-40-6 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1R)-1-[[(1,1-1)]]

dimethylethoxy)carbonyl]amino]-

3-(4-nitrophenoxy)propyl]phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 444646-49-5 CAPLUS

CN Benzoic acid, 4-[3-[4-[[(dimethylamino)carbonyl]oxy]phenyl]-3[methyl[(phenylmethoxy)carbonyl]amino]propoxy]- (9CI) (CA INDEX NAME)

RN 444646-61-1 CAPLUS

CN Carbamic acid, dimethyl-, (1R)-1-[2-(4-chloro-3-methylphenyl)ethyl]-1,2,3,4-tetrahydro-2-(trifluoroacetyl)-6-isoquinolinyl ester (9CI)

(CA

INDEX NAME)

Absolute stereochemistry.

444646-82-6 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1R)-1-amino-3-[4-

(methylthio) phenoxy]propyl]-

3-hydroxyphenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN444646-83-7 CAPLUS

Carbamic acid, dimethyl-, 4-[(1R)-1-[[(1,1-

dimethylethoxy)carbonyl]amino]-

3-[4-(methylthio)phenoxy]propyl]-3-hydroxyphenyl ester (9CI) (CA

INDEX

NAME)

Absolute stereochemistry.

RN 444646-84-8 CAPLUS

Carbamic acid, dimethyl-, 4-[(1R)-1-[[(1,1-

dimethylethoxy)carbonyl]amino]-

3-[4-(methylthio)phenoxy]propyl]-3-ethenylphenyl ester (9CI) (CA INDEX

NAME)

Absolute stereochemistry.

RN 444646-85-9 CAPLUS

CN Carbamic acid, dimethyl-, 4-[(1R)-1-[[(1,1-dimethylethoxy)carbonyl]-2-propenylamino]-3-[4-(methylthio)phenoxy]propyl]-3-ethenylphenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 444646-86-0 CAPLUS

CN 2H-2-Benzazepine-2-carboxylic acid, 7-[[(dimethylamino)carbonyl]oxy]1,3-

dihydro-1-[2-[4-(methylthio)phenoxy]ethyl]-, 1,1-dimethylethyl ester, (1R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 444646-89-3 CAPLUS

CN Methanesulfonic acid, trifluoro-, 5-[[(dimethylamino)carbonyl]oxy]-2-[(1R)-

1-[[(1,1-dimethylethoxy)carbonyl]amino]-3-[4(methylthio)phenoxy]propyl]ph

enyl ester (9CI) (CA INDEX NAME)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 6 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2001:196132 CAPLUS Full-text

DN 135:2935

TI Tetrahydroisoquinoline-monoterpene and iridoid glycosides from Alanqium

lamarckii

AU Itoh, A.; Tanahashi, T.; Tabata, M.; Shikata, M.; Kakite, M.; Nagai, M.;

Nagakura, N.

CS Kobe Pharmaceutical University, Higashinada-ku, Kobe, 658-8558, Japan

SO Phytochemistry (2001), 56(6), 623-630 CODEN: PYTCAS; ISSN: 0031-9422

PB Elsevier Science Ltd.

DT Journal

LA English

IT 342036-89-9P 342036-90-2P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and properties of)

RN 342036-89-9 CAPLUS

CN 2H-Pyran-5-carboxylic acid, $4-[[(1S)-2-acetyl-7-(acetyloxy)-1,2,3,4-tetrahydro-6-methoxy-1-isoquinolinyl]methyl]-3-ethenyl-3,4-dihydro-2-[(2,3,4,6-tetra-0-acetyl-<math>\beta$ -D-glucopyranosyl)oxy]-, (2S,3R,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A

PAGE 2-A

RN 342036-90-2 CAPLUS

CN 2H-Pyran-5-carboxylic acid, $4-[(1S)-2-acetyl-6-(acetyloxy)-1,2,3,4-tetrahydro-7-methoxy-1-isoquinolinyl]methyl]-3-ethenyl-3,4-dihydro-2-[(2,3,4,6-tetra-0-acetyl-<math>\beta$ -D-glucopyranosyl)oxy]-, (2S,3R,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 2-A

RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 7 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2000:172231 CAPLUS Full-text

DN 132:305767

TI A tetrahydroisoquinoline-monoterpene glucoside and an iridoid

glucoside

from Alangium kurzii

- AU Tanahashi, Takao; Kobayashi, Chizu; Itoh, Atsuko; Nagakura, Naotaka; Inoue, Kenichiro; Kuwajima, Hiroshi; Wu, Hua-Xin
- CS Kobe Pharmaceutical University, Kobe, 658-8558, Japan
- SO Chemical & Pharmaceutical Bulletin (2000), 48(3), 415-419 CODEN: CPBTAL; ISSN: 0009-2363
- PB Pharmaceutical Society of Japan
- DT Journal
- LA English
- IT 137318-71-9P 265096-94-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and properties of)

- RN 137318-71-9 CAPLUS
- CN 2H-Pyran-5-carboxylic acid, $4-[[(1R)-2-acetyl-7-(acetyloxy)-1,2,3,4-tetrahydro-6-methoxy-1-isoquinolinyl]methyl]-3-ethenyl-3,4-dihydro-2-[(2,3,4,6-tetra-0-acetyl-<math>\beta$ -D-glucopyranosyl)oxy]-, methyl ester, (2S,3R,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A

PAGE 2-A

- RN 265096-94-4 CAPLUS
- CN 2H-Pyran-5-carboxylic acid, $4-[[(1R)-2-acetyl-7-(acetyloxy)-1,2,3,4-tetrahydro-6-methoxy-1-isoquinolinyl]methyl]-3-ethenyl-3,4-dihydro-2-[(2,3,4,6-tetra-0-acetyl-<math>\beta$ -D-glucopyranosyl)oxy]-, (2S,3R,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 2-A

RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 8 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1997:303161 CAPLUS Full-text

DN 127:50579

TI Oxazepines and Thiazepines. Part 33. An efficient procedure for the preparation of 3-acetyl-2,3-dihydrobenzothiazoles by ring contraction of

 ${\tt 2,4-diaryl-2,3-dihydro-1,5-benzothiazepines\ under\ acetylating\ conditions}$

AU Toth, Gabor; Levai, Albert; Balazs, Barbara; Simon, Andras

CS Technical Analytical Research Group, Hungarian Academy Sciences, Budapest,

H-1111, Hung.

SO Liebigs Annalen/Recueil (1997), (5), 995-998

CODEN: LIARFV

PB VCH

DT Journal

LA English

OS CASREACT 127:50579

IT 191017-21-7P 191017-23-9P 191017-24-0P 191017-25-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of acetyldihydrobenzothiazoles by ring contraction of aryldihydrobenzothiazepines under acetylating conditions)

RN 191017-21-7 CAPLUS

CN Benzothiazole, 3-acetyl-2-[4-(acetyloxy)phenyl]-2,3-dihydro-2-[(1E)-2-phenylethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 191017-23-9 CAPLUS

CN Benzothiazole, 3-acetyl-2-[2-(acetyloxy)phenyl]-2,3-dihydro-2-[(1E)-2-phenylethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 191017-24-0 CAPLUS

CN Benzothiazole, 3-acetyl-2-[2-(acetyloxy)-4-methoxyphenyl]-2,3-dihydro-2-(2-

phenylethenyl)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 191017-25-1 CAPLUS

CN Benzothiazole, 3-acetyl-2-[2-(acetyloxy)phenyl]-2,3-dihydro-2-[2-(4-methoxyphenyl)ethenyl]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

- L16 ANSWER 9 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN
- AN 1996:582453 CAPLUS Full-text
- DN 125:243101
- TI Berberis alkaloids. XXXIV. Turcomanine, a new alkaloid from Berberis turcomanica
- AU Khamidov, I.; Faskhutdinov, M.; Telezhenetskaya, M. V.; Karimov, A.; Levkovich, M. G.; Abdullaev, N. D.; Shakirov, R. Sh.
- CS Inst. Khim. Rastit. Veshchestv, Tashkent, Uzbekistan
- SO Khimiya Prirodnykh Soedinenii (1996), (1), 74-76 CODEN: KPSUAR; ISSN: 0023-1150
- PB Fan
- DT Journal
- LA Russian
- RN 182121-11-5 CAPLUS
- CN 1,2-Benzenediol, 4-[[7-(acetyloxy)-6-methoxy-1-isoquinolinyl]methyl]-, diacetate (ester) (9CI) (CA INDEX NAME)

- L16 ANSWER 10 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN
- AN 1996:560528 CAPLUS Full-text
- DN 125:195213
- TI Preparation of 2-(aryl or heterocyclyl)-1-phenylethylamine derivatives
- as
 - δ -opioid receptor agonists
- IN Murase, Masao; Hamada, Kozo; Asaki, Tetsuo
- PA Nippon Shinyaku Co., Ltd., Japan
- SO PCT Int. Appl., 93 pp.
- CODEN: PIXXD2
- DT Patent
- LA Japanese
- FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE --------------_____ WO 9622276 PΤ A119960725 WO 1996-JP86 19960119 W: AU, BR, CA, CN, FI, HU, JP, KR, MX, NO, NZ, RU, UA, US, VN, ΑZ, BY, KG, KZ, RU, TJ, TM RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE AU 9644589 A1 19960807 AU 1996-44589 19960119 PRAI JP 1995-7670 19950120 WO 1996-JP86 19960119 OS MARPAT 125:195213 IΤ 181069-29-4P 181069-30-7P 181069-31-8P 181069-32-9P 181069-33-0P 181069-34-1P 181069-35-2P 181069-36-3P 181069-37-4P 181069-39-6P 181069-40-9P 181069-41-0P 181069-42-1P 181069-43-2P RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of (phenylethyl)amine derivs. as δ -opioid receptor agonists as analgesics and immunostimulants and for treating frequent urination and urinary incontinence) RN 181069-29-4 CAPLUS CN Phenol, 3-[1-(dimethylamino)-2-(2-naphthalenyl)ethyl]-, acetate (ester), hydrochloride, (+) - (9CI) (CA INDEX NAME)

OAc NMe2

HC1

Rotation (+).

Rotation (+).

OAc

RN 181069-31-8 CAPLUS

CN Benzoic acid, 4-[2-[3-(acetyloxy)phenyl]-2-(dimethylamino)ethyl]-, ethyl ester, hydrochloride (9CI) (CA INDEX NAME)

HC1

RN 181069-32-9 CAPLUS
CN 1-Propanone, 1-[4-[2-[3-(acetyloxy)phenyl]-2-(dimethylamino)ethyl]phenyl], hydrochloride (9CI) (CA INDEX NAME)

● HCl

● HCl

RN 181069-35-2 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, 3-[1-(dimethylamino)-2-(2-naphthalenyl)ethyl]phenyl ester, hydrochloride, (+)- (9CI) (CA INDEX NAME)

Rotation (+).

HCl

RN 181069-36-3 CAPLUS

INDEX NAME)

Rotation (+).

● HCl

RN 181069-37-4 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, 3-[1-(dimethylamino)-2-[4-(ethoxymethyl)phenyl]ethyl]phenyl ester, hydrochloride, (+)- (9CI) (CA

INDEX NAME)

Rotation (+).

RN 181069-39-6 CAPLUS

CN Carbamic acid, propyl-, 3-[1-(dimethylamino)-2-[4-(ethoxymethyl)phenyl]ethyl]phenyl ester, monohydrochloride, (+)- (9CI) (CA INDEX NAME)

Rotation (+).

HC1

RN 181069-40-9 CAPLUS

CN Carbamic acid, propyl-, 3-[1-(dimethylamino)-2-[4-(ethoxymethyl)phenyl]ethyl]phenyl ester, (+)- (9CI) (CA INDEX NAME)

Rotation (+).

RN 181069-41-0 CAPLUS

Rotation (+).

RN 181069-42-1 CAPLUS

CN Carbamic acid, dimethyl-, 3-[1-(dimethylamino)-2-[4-(ethoxymethyl)phenyl]ethyl]phenyl ester, (+)- (9CI) (CA INDEX NAME)

Rotation (+).

RN 181069-43-2 CAPLUS

Rotation (+).

● HCl

L16 ANSWER 11 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1995:982327 CAPLUS Full-text

DN 124:55796

TI Preparation of nonpeptide heterocyclic amides as neurokinin A antagonists

IN Shenvi, Ashokkumar Bhikkappa; Jacobs, Robert Toms; Miller, Scott
Carson;

Ohnmacht, Cyrus John, Jr.; Veale, Chris Allan

PA Zeneca Ltd., UK

SO PCT Int. Appl., 157 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN. CNT 1

	PAT	ENT :	NO.		KII		DATE		APPLICATION NO. DATE									
PI	WO				A1		19950622			WO 1994-GB2726 1994121								
		w:	AM,	ΑT,	AU,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CZ,	DE,	DK,	ES,	FI,	
GB,									***		T 7.	T M	T 11	T 1.F	MD	MC	MAT	
3.67			GE,	HU,	JP,	KE,	KG,	KP,	KK,	ĸz,	LК,	LT,	ъо,	цν,	MD,	MG,	Ми,	
MW,			NT.	NO	NZ	PT.	PT,	RO.	RU.	SD.	SE.	SI.	SK.	TJ.	TT.	UA,	UZ,	VN
		RW:	KE.	MW.	SD.	SZ.	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IE,	IT,	
LU,		•	,	,		,			•	•	·	•	•		·			
			MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	ML,	MR,	ΝE,	
SN,																		
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		5589					1996					94-3			1994			
	ZA 9409934 CA 2176036					19950615 19950622			ZA 1994-9934 19941213 CA 1994-2176036 19941213									
					A	_						94-2 95-1						
		9512			Α.		1995			A	0 19	95-1	24/I		1994	1213		
		6909			В:		1998			_	- 10	٥- ٥	0041	_	1004	1010		
		7343					1996			E.	Ь 19	95-9	0341	5	1994	1213		
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	a.D	R:	AT,	BE,	CH,	DE,	DK,	ES,	FK,	GD,	GR,	IE,	II,	ът,	ьо,	MC,	мъ,	
PT,		1110	000		7		1007	0212		C	NT 10	94-1	0101	1	1994	1213		
		1142			A		1997 1997					96-1		7	1994			
		7627			A:							94-8			1994			
		9408			A		1997					94-0			1994			
		1119			A		1999					95-9			1994			
		2210			E		2002					95-9			1994			
		2179			T		2003					96-2			1996			
		9602			A		1996					96-2			1996			
		9602			A A		1996								1996			
		5705			A A		1998 1999								1997			
DDAT		5965		5.4			1993			U	3 19	31-3	0033	,	1991	1120		
PRAI		1993 1994			-		1994											
		1994			A A		1994											
		1994			W		1994											
		1996			A.		1996											
os						,	1550	0 2 2 0										
IT	MARPAT 124:55796 171426-11-2P																	
11		RCT			nt):	SPN	J (Sv	nthe	tic	prep	arat	ion)	; PR	EP (Prep	arat	ion)	;
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anta	gon	ists)	P				-											
RN	-		11-2	CA	PLUS													
CN	171426-11-2 CAPLUS 1H-Isoindol-1-one, 6-(acetyloxy)-3-[1-(3,4-dichlorophenyl)-3-butenyl]-																	
2,3-															_			
•		hydro	-2-m	ethy	1-,	(R*,	s*)-	(9C	I)	(CA	INDE	X NA	ME)					

Relative stereochemistry.

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L16 ANSWER 12 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN
AN
    1995:451708 CAPLUS Full-text
    122:214056
DN
    preparation of 1,2-benzisoxazole derivatives and salts as brain
TI
protective
    agents
    Takeda, Kenji; Terashima, Nobuo; Nakano, Joji; Minami, Hisashi;
IN
Kobayashi,
    Toyokazu; Furuhata, Kunikazu; Takakura, Tadakazu; Takata, Makoto;
    Kawafuchi, Hiroyo; Hiraiwa, Toru
    Toyama Chemical Co., Ltd., Japan
PA
    PCT Int. Appl., 173 pp.
SO
    CODEN: PIXXD2
DΤ
    Patent
LA
     Japanese
FAN.CNT 1
                                         APPLICATION NO. DATE
    PATENT NO.
                     KIND DATE
                                          _____
     _____ ----
                      A1
                           19940511
                                          WO 1993-JP1549
                                                          19931027
PI
    WO 9410158
        W: AU, CA, JP, KR, US
        RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
                                                          19931027
                           19940524
                                         AU 1994-53442
    AU 9453442
                      A1
                           19961219
    AU 674358
                      B2
                                         EP 1993-923647
                                                         19931027
                           19950802
    EP 665226
                      A1
        R: BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, NL, SE
                                         JP 1994-510885 19931027
     JP 3457669
                     B2
                           20031020
                                          US 1995-411667
                                                          19950412
    US 5578627
                      Α
                           19961126
PRAI JP 1992-312743
                     Α
                           19921028
                           19930702
                     Α
     JP 1993-238688
                           19930715
     JP 1993-197776
                      Α
                           19931027
                      W
    WO 1993-JP1549
os
    MARPAT 122:214056
    162035-09-8P 162035-11-2P
     RL: BAC (Biological activity or effector, except adverse); BSU
(Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic
use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of 1,2-benzisoxazole derivs. and salts as brain
protective
        agents)
RN
     162035-09-8 CAPLUS
     Phenol, 3-[1-amino-2-[(5-chloro-1,2-benzisoxazol-3-yl)oxy]ethyl]-,
CN
     carbamate (ester), monohydrochloride (9CI) (CA INDEX NAME)
                          NH2
```

RN 162035-11-2 CAPLUS

HCl

CN Phenol, 4-[1-amino-2-[(5-chloro-1,2-benzisoxazol-3-yl)oxy]ethyl]-, carbamate (ester), monohydrochloride (9CI) (CA INDEX NAME)

L16 ANSWER 13 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN 1994:478365 CAPLUS Full-text AN121:78365 DN Tetrahydroisoquinoline-monoterpene glucosides from Alangium lamarckii ΤI and Cephaelis ipecacuanha Itoh, Atsuko; Tanahashi, Takao; Nagakura, Naotaka; Nayeshiro, Hidekazu ΑU Kobe Women's Coll. Pharm., Kobe, 658, Japan CS Phytochemistry (1994), 36(2), 383-7 CODEN: PYTCAS; ISSN: 0031-9422 \mathbf{DT} Journal LA English 156366-69-7P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) 156366-69-7 CAPLUS RN2H-Pyran-5-carboxylic acid, 4-[[2-acetyl-6-(acetyloxy)-1,2,3,4-CN tetrahydro-7-methoxy-1-isoquinolinyl]methyl]-3-ethenyl-3,4-dihydro-2-[(2,3,4,6- $O-acetyl-\beta-D-glucopyranosyl)oxy]-$, methyl ester, [2S- $[2\alpha, 3\beta, 4\beta(S^*)]$ (9CI) (CA INDEX NAME)

L16 ANSWER 14 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN AN 1994:245566 CAPLUS Full-text

DN 120:245566

TI General asymmetric synthesis of isoquinoline alkaloids.

Enantioselective

hydrogenation of enamides catalyzed by BINAP-ruthenium(II) complexes U Kitamura, Masato; Hsiao, Yi; Ohta, Masako; Tsukamoto, Masaki; Ohta, Tetsuo; Takaya, Hidemasa; Noyori, Ryoji CS Dep. Chem., Nagoya Univ., Chikusa, 464-01, Japan SO Journal of Organic Chemistry (1994), 59(2), 297-310 CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

LA English

OS CASREACT 120:245566

IT 104621-45-6 104621-46-7

RL: RCT (Reactant); RACT (Reactant or reagent) (intermediate, synthesis of isoquinoline alkaloid)

RN 104621-45-6 CAPLUS

CN 7-Isoquinolinol, 2-acetyl-1-[[3-(acetyloxy)-4-methoxyphenyl]methyl]-1,2,3,4-tetrahydro-6-methoxy-, acetate (ester), (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 104621-46-7 CAPLUS

CN 7-Isoquinolinol, 2-acetyl-1-[[3-(acetyloxy)-4-methoxyphenyl]methyl]-1,2,3,4-tetrahydro-6-methoxy-, acetate (ester), (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L16 ANSWER 15 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1994:106723 CAPLUS Full-text

DN 120:106723

TI Enzymic resolution of acylates of prochiral phenolic 1-aryl- and 1-arylalkyl-1,2,3,4-tetrahydroisoquinolinols, which possess a guaiacol-type moiety, by use of immobilized lipase in organic solvent AU Hoshino, Osamu; Tanahashi, Ruka; Okada, Mitsuhiro; Akita, Hiroyuki; Oishi,

Takeshi

CS Fac. Pharm. Sci., Sci. Univ. Tokyo, Tokyo, 162, Japan

SO Tetrahedron: Asymmetry (1993), 4(5), 933-42

CODEN: TASYE3; ISSN: 0957-4166

DT Journal

LA English

OS CASREACT 120:106723

IT 152561-05-2 152561-06-3 152561-07-4

152561-08-5 152561-09-6 152561-10-9

152561-18-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(enzymic resolution of)

RN 152561-05-2 CAPLUS

CN 5-Isoquinolinol, 1-[(3,4-dimethoxyphenyl)methyl]-1,2,3,4-tetrahydro-6-

methoxy-2-methyl-, acetate (ester) (9CI) (CA INDEX NAME)

RN 152561-06-3 CAPLUS

CN 6-Isoquinolinol, 1-[(3,4-dimethoxyphenyl)methyl]-1,2,3,4-tetrahydro-7-methoxy-2-methyl-, acetate (ester) (9CI) (CA INDEX NAME)

RN 152561-07-4 CAPLUS

CN 7-Isoquinolinol, 1-[(3,4-dimethoxyphenyl)methyl]-1,2,3,4-tetrahydro-6-methoxy-2-methyl-, acetate (ester) (9CI) (CA INDEX NAME)

RN 152561-08-5 CAPLUS
CN 5-Isoquinolinol, 1-[2-(3,4-dimethoxyphenyl)ethyl]-1,2,3,4-tetrahydro6methoxy-2-methyl-, acetate (ester) (9CI) (CA INDEX NAME)

RN 152561-09-6 CAPLUS
CN 6-Isoquinolinol, 1-[2-(3,4-dimethoxyphenyl)ethyl]-1,2,3,4-tetrahydro7methoxy-2-methyl-, acetate (ester) (9CI) (CA INDEX NAME)

RN 152561-10-9 CAPLUS
CN 7-Isoquinolinol, 1-[2-(3,4-dimethoxyphenyl)ethyl]-1,2,3,4-tetrahydro6methoxy-2-methyl-, acetate (ester) (9CI) (CA INDEX NAME)

RN 152561-18-7 CAPLUS

CN 6-Isoquinolinol, 1-(1,3-benzodioxol-5-ylmethyl)-1,2,3,4-tetrahydro-7-methoxy-2-methyl-, acetate (ester) (9CI) (CA INDEX NAME)

IT 152693-96-4P 152693-97-5P 152693-98-6P 152693-99-7P 152694-00-3P 152694-01-4P 152694-02-5P 152694-03-6P 152694-04-7P 152694-05-8P 152694-06-9P 152694-07-0P

152694-18-3P 152694-19-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 152693-96-4 CAPLUS

CN 5-Isoquinolinol, 1-[(3,4-dimethoxyphenyl)methyl]-1,2,3,4-tetrahydro-6-methoxy-2-methyl-, acetate (ester), (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 152693-97-5 CAPLUS

CN 5-Isoquinolinol, 1-[(3,4-dimethoxyphenyl)methyl]-1,2,3,4-tetrahydro-6-methoxy-2-methyl-, acetate (ester), (S)- (9CI) (CA INDEX NAME)

RN 152693-98-6 CAPLUS

CN 6-Isoquinolinol, 1-[(3,4-dimethoxyphenyl)methyl]-1,2,3,4-tetrahydro-7-methoxy-2-methyl-, acetate (ester), (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 152693-99-7 CAPLUS

CN 6-Isoquinolinol, 1-[(3,4-dimethoxyphenyl)methyl]-1,2,3,4-tetrahydro-7-methoxy-2-methyl-, acetate (ester), (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 152694-00-3 CAPLUS

CN 7-Isoquinolinol, 1-[(3,4-dimethoxyphenyl)methyl]-1,2,3,4-tetrahydro-6-methoxy-2-methyl-, acetate (ester), (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 152694-01-4 CAPLUS

CN 7-Isoquinolinol, 1-[(3,4-dimethoxyphenyl)methyl]-1,2,3,4-tetrahydro-6-methoxy-2-methyl-, acetate (ester), (S)- (9CI) (CA INDEX NAME)

RN 152694-02-5 CAPLUS
CN 5-Isoquinolinol, 1-[2-(3,4-dimethoxyphenyl)ethyl]-1,2,3,4-tetrahydro6methoxy-2-methyl-, acetate (ester), (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 152694-03-6 CAPLUS
CN 5-Isoquinolinol, 1-[2-(3,4-dimethoxyphenyl)ethyl]-1,2,3,4-tetrahydro6methoxy-2-methyl-, acetate (ester), (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 152694-04-7 CAPLUS CN 6-Isoquinolinol, 1-[2-(3,4-dimethoxyphenyl)ethyl]-1,2,3,4-tetrahydro-7methoxy-2-methyl-, acetate (ester), (R)- (9CI) (CA INDEX NAME)
Absolute stereochemistry.

RN 152694-05-8 CAPLUS
CN 6-Isoquinolinol, 1-[2-(3,4-dimethoxyphenyl)ethyl]-1,2,3,4-tetrahydro7methoxy-2-methyl-, acetate (ester), (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 152694-06-9 CAPLUS
CN 7-Isoquinolinol, 1-[2-(3,4-dimethoxyphenyl)ethyl]-1,2,3,4-tetrahydro6methoxy-2-methyl-, acetate (ester), (R)- (9CI) (CA INDEX NAME)

RN 152694-07-0 CAPLUS
CN 7-Isoquinolinol, 1-[2-(3,4-dimethoxyphenyl)ethyl]-1,2,3,4-tetrahydro6methoxy-2-methyl-, acetate (ester), (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 152694-18-3 CAPLUS

CN 6-Isoquinolinol, 1-(1,3-benzodioxol-5-ylmethyl)-1,2,3,4-tetrahydro-7-methoxy-2-methyl-, acetate (ester), (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 152694-19-4 CAPLUS

CN 6-Isoquinolinol, 1-(1,3-benzodioxol-5-ylmethyl)-1,2,3,4-tetrahydro-7-methoxy-2-methyl-, acetate (ester), (S)- (9CI) (CA INDEX NAME)

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L16 ANSWER 16 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN
     1993:445228 CAPLUS Full-text
AN
     119:45228
DN
     Four tetrahydroisoquinoline-monoterpene glucosides from Cephaelis
TI
     ipecacuanha
     Nagakura, Naotaka; Itoh, Atsuko; Tanahashi, Takao
ΑU
     Kobe Women's Coll. Pharm., Kobe, 658, Japan
CS
     Phytochemistry (1993), 32(3), 761-5
SO
     CODEN: PYTCAS; ISSN: 0031-9422
DΤ
     Journal
LA
     English
     21104-39-2, Ipecoside hexaacetate
IT
     RL: BIOL (Biological study)
        (cephaloside heptaacetate preparation from)
     21104-39-2 CAPLUS
RN
     2H-Pyran-5-carboxylic acid, 4-[[2-acetyl-6,7-bis(acetyloxy)-1,2,3,4-
     tetrahydro-1-isoquinolinyl]methyl]-3-ethenyl-3,4-dihydro-2-[(2,3,4,6-
tetra-
     O-acetyl-\beta-D-glucopyranosyl)oxy]-, methyl ester, [2S-
     [2\alpha, 3\beta, 4\beta(s^*)] (9CI) (CA INDEX NAME)
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AcO OAC OAC OAC
$$H_2C$$
 CH C OMe C A C

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L16 ANSWER 17 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN
    1992:105914 CAPLUS Full-text
AN
DN
     116:105914
    Reactions of flavonoid thiosemicarbazones under acetylating conditions
TΙ
     Somogyi, Laszlo
ΑU
     Res. Group Antibiot., Hung. Acad. Sci., Debrecen, H-4010, Hung.
CS
     Tetrahedron (1991), 47(44), 9305-16
SO
     CODEN: TETRAB; ISSN: 0040-4020
DT
     Journal
     English
LA
     139061-57-7P
IT
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of, from thiosemicarbazone)
     139061-57-7 CAPLUS
RN
     Acetamide, N-[4-acetyl-5-[2-(acetyloxy)phenyl]-4,5-dihydro-5-(2-
CN
     phenylethenyl)-1,3,4-thiadiazol-2-yl]-, (E)- (9CI) (CA INDEX NAME)
```

Double bond geometry as shown.

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ANSWER 18 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN
L16
ΑN
    1991:652125 CAPLUS Full-text
DN
    115:252125
    Six tetrahydroisoquinoline-monoterpene glucosides from Cephaelis
ΤI
    ipecacuanha
    Itoh, Atsuko; Tanahashi, Takao; Nagakura, Naotaka
ΑU
    Kobe Women's Coll. Pharm., Kobe, 658, Japan
CS
    Phytochemistry (1991), 30(9), 3117-23
SO
    CODEN: PYTCAS; ISSN: 0031-9422
DT
    Journal
LA
    English
    21104-39-2
IT
    RL: RCT (Reactant); RACT (Reactant or reagent)
       (cyclization of)
RN
    21104-39-2 CAPLUS
```

O-acetyl- β -D-glucopyranosyl)oxy]-, methyl ester, [2S-[2 α , 3 β , 4 β (S*)]]- (9CI) (CA INDEX NAME)

IT 122587-80-8P 137318-71-9P 137318-72-0P 137318-75-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, by acetylation of alkaloidal glycoside from Cephaelis

ipecacuanha)

RN 122587-80-8 CAPLUS

CN 2H-Pyran-5-carboxylic acid, 4-[[2-acetyl-8-(acetyloxy)-1,2,3,4-tetrahydro-

7-methoxy-1-isoquinolinyl]methyl]-3-ethenyl-3,4-dihydro-2-[(2,3,4,6-tetra-

O-acetyl- β -D-glucopyranosyl)oxy]-, methyl ester, [2S-[2 α , 3 β , 4 β (S*)]]- (9CI) (CA INDEX NAME)

RN 137318-71-9 CAPLUS

CN 2H-Pyran-5-carboxylic acid, $4-[[(1R)-2-acetyl-7-(acetyloxy)-1,2,3,4-tetrahydro-6-methoxy-1-isoquinolinyl]methyl]-3-ethenyl-3,4-dihydro-2-[(2,3,4,6-tetra-O-acetyl-<math>\beta$ -D-glucopyranosyl)oxy]-, methyl ester, (2S,3R,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A

PAGE 2-A

RN 137318-72-0 CAPLUS

CN 2H-Pyran-5-carboxylic acid, 4-[[2-acetyl-6,7-bis(acetyloxy)-1,2,3,4-tetrahydro-1-isoquinolinyl]methyl]-3-ethenyl-3,4-dihydro-2-[(2,3,4,6-tetra-

O-acetyl- β -D-glucopyranosyl)oxy]-, [2S-[2 α , 3 β , 4 β (S*)]]- (9CI) (CA INDEX NAME)

$$AcO-CH_2$$
 H_2C
 CH
 CO_2H
 AcO
 AcO
 AcO
 AcO

RN 137318-75-3 CAPLUS

CN 2H-Pyran-5-carboxylic acid, 4-[[2-acetyl-7,8-bis(acetyloxy)-1,2-dihydro-1-

 $isoquinolinyl] \verb|methyl|-3-ethenyl-3|, 4-dihydro-2-[(2,3,4,6-tetra-0-acetyl-a$

 β -D-glucopyranosyl)oxy]-, methyl ester, [2S-

$[2\alpha, 3\beta, 4\beta(S^*)]$ (9CI) (CA INDEX NAME)

IT 122587-78-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, by acetylation of alkaloidal glycoside from Cephaelis

ipecacuanha, and cyclization of)

RN 122587-78-4 CAPLUS

CN 2H-Pyran-5-carboxylic acid, 4-[[2-acetyl-7,8-bis(acetyloxy)-1,2,3,4-tetrahydro-1-isoquinolinyl]methyl]-3-ethenyl-3,4-dihydro-2-[(2,3,4,6-tetra-

O-acetyl- β -D-glucopyranosyl)oxy]-, methyl ester, [2S-[2 α , 3 β , 4 β (S*)]]- (9CI) (CA INDEX NAME)

L16 ANSWER 19 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1991:450035 CAPLUS Full-text

DN 115:50035

TI Revised stereostructure for (+)-roemecarine and synthesis of (\pm) -, (+)-, and (-)-roemecarine and (\pm) -epiroemecarine

AU Hoshino, Osamu; Itoh, Katsuhiko; Tanahashi, Ruka; Umezawa, Bunsuke; Akita,

Hiroyuki; Oishi, Takeshi

CS Fac. Pharm. Sci., Sci. Univ. Tokyo, Tokyo, 162, Japan

SO Chemical & Pharmaceutical Bulletin (1990), 38(12), 3277-9 CODEN: CPBTAL; ISSN: 0009-2363

DT Journal

LA English

OS CASREACT 115:50035

IT 96012-67-8

RL: PROC (Process)

(enzymic kinetic resolution of)

RN 96012-67-8 CAPLUS

CN 4,6-Isoquinolinediol, 1-[(3,4-dimethoxyphenyl)methyl]-1,2,3,4-tetrahydro-7-

methoxy-2-methyl-, diacetate (ester), trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L16 ANSWER 20 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1991:229209 CAPLUS Full-text

DN 114:229209

TI The structure and partial synthesis of imbricatine, a benzyltetrahydroisoquinoline alkaloid from the starfish Dermasterias imbricata

AU Burgoyne, David L.; Miao, Shichang; Pathirana, Charles; Andersen, Raymond

J.; Ayer, William A.; Singer, Peter P.; Kokke, William C. M. C.; Ross, Donald M.

CS Dep. Chem., Univ. British Columbia, Vancouver, BC, V6T 1W5, Can.

SO Canadian Journal of Chemistry (1991), 69(1), 20-7 CODEN: CJCHAG; ISSN: 0008-4042

DT Journal

LA English

OS CASREACT 114:229209

IT 105372-71-2P 133761-47-4P 133761-48-5P

133761-56-5P 133761-57-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 105372-71-2 CAPLUS

CN 3-Isoquinolinecarboxylic acid, 2-acetyl-5-[[5-[2-(acetylamino)-3-methoxy-3-

oxopropyl]-1-methyl-1H-imidazol-4-yl]thio]-6,8-bis(acetyloxy)-1-[[4-(acetyloxy)phenyl]methyl]-1,2,3,4-tetrahydro-, methyl ester, [1R-[1 α ,3 α ,5(S*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 133761-47-4 CAPLUS

CN 3-Isoquinolinecarboxylic acid, 2-acetyl-6,7-bis(acetyloxy)-1,2,3,4-tetrahydro-1-[(4-methoxyphenyl)methyl]-, methyl ester, (1S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 133761-48-5 CAPLUS

CN 3-Isoquinolinecarboxylic acid, 2-acetyl-6,7-bis(acetyloxy)-1,2,3,4tetrahydro-1-[(4-methoxyphenyl)methyl]-, methyl ester, (1R-trans)(9CI)

(CA INDEX NAME)

Absolute stereochemistry.

RN 133761-56-5 CAPLUS

CN 3-Isoquinolinecarboxylic acid, 2-acetyl-6,8-bis(acetyloxy)-1-[[4-(acetyloxy)phenyl]methyl]-1,2,3,4-tetrahydro-, methyl ester, cis-

(9CI)

(CA INDEX NAME)

Relative stereochemistry.

RN 133761-57-6 CAPLUS

CN 3-Isoquinolinecarboxylic acid, 2-acetyl-6,8-bis(acetyloxy)-1-[[4-(acetyloxy)phenyl]methyl]-1,2,3,4-tetrahydro-, methyl ester, trans-(9CI)

(CA INDEX NAME)

Relative stereochemistry.

IT 133761-54-3P 133761-55-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

RACT

(Reactant or reagent)

(preparation, hydrogenolysis, and acetylation of)

RN 133761-54-3 CAPLUS

CN 3-Isoquinolinecarboxylic acid, 2-acetyl-6,8-bis(acetyloxy)-1,2,3,4tetrahydro-1-[[4-(phenylmethoxy)phenyl]methyl]-, methyl ester, cis(9CI)

(CA INDEX NAME)

RN 133761-55-4 CAPLUS

CN 3-Isoquinolinecarboxylic acid, 2-acetyl-6,8-bis(acetyloxy)-1,2,3,4-tetrahydro-1-[[4-(phenylmethoxy)phenyl]methyl]-, methyl ester, trans-(9CI) (CA INDEX NAME)

Relative stereochemistry.

L16 ANSWER 21 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1991:98333 CAPLUS Full-text

DN 114:98333

TI The biosynthesis of the phenethylisoquinoline alkaloid colchicine. Early

and intermediate stages

AU Herbert, Richard B.; Kattah, Abdullah E.; Knagg, Eric

CS Sch. Chem., Univ. Leeds, Leeds, LS2 9JT, UK

SO Tetrahedron (1990), 46(20), 7119-38

CODEN: TETRAB; ISSN: 0040-4020

DT Journal

LA English

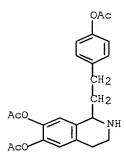
IT 131946-66-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 131946-66-2 CAPLUS

CN 6,7-Isoquinolinediol, 1-[2-[4-(acetyloxy)phenyl]ethyl]-1,2,3,4-tetrahydro-

, diacetate (ester) (9CI) (CA INDEX NAME)



L16 ANSWER 22 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1990:156714 CAPLUS Full-text

DN 112:156714

TI Enzymic resolution of isoquinoline alkaloids

IN Oishi, Takeshi; Umezawa, Fumisuke; Hoshino, Osamu; Akita, Hiroyuki; Machida, Haruo

PA Institute of Physical and Chemical Research, Japan; Meito Sangyo Co., Ltd.

SO Jpn. Kokai Tokkyo Koho, 7 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
		-			
ΡI	JP 01228964	A 2	19890912	JP 1988-56887	19880310
PRAI	JP 1988-56887		19880310		

IT 96012-67-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

RACT

(Reactant or reagent)

(preparation and enzymic resolution of)

RN 96012-67-8 CAPLUS

CN 4,6-Isoquinolinediol, 1-[(3,4-dimethoxyphenyl)methyl]-1,2,3,4-tetrahydro-7-

methoxy-2-methyl-, diacetate (ester), trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

IT 125942-07-6P

RL: PREP (Preparation)

(preparation of, via enzymic resolution)

RN 125942-07-6 CAPLUS

CN 4,6-Isoquinolinediol, 1-[(3,4-dimethoxyphenyl)methyl]-1,2,3,4-tetrahydro-7-

methoxy-2-methyl-, diacetate (ester), trans-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.

L16 ANSWER 23 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1990:18869 CAPLUS Full-text

DN 112:18869

TI Neoipecoside and 7-methylneoipecoside, new unusually-cyclized tetrahydroisoquinoline-monoterpene glucosides from Cephaelis ipecacuanha

[Erratum to document cited in CA111(15):130718m]

AU Itoh, Atsuko; Tanahashi, Takao; Nagakura, Naotaka

CS Kobe Women's Coll. Pharm., Kobe, 658, Japan

SO Chemical & Pharmaceutical Bulletin (1989), 37(6), 1684 CODEN: CPBTAL; ISSN: 0009-2363

DT Journal

LA English

IT 122587-78-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

RACT

(Reactant or reagent)

(preparation and deacetylation of (Erratum))

RN 122587-78-4 CAPLUS

CN 2H-Pyran-5-carboxylic acid, 4-[[2-acetyl-7,8-bis(acetyloxy)-1,2,3,4-tetrahydro-1-isoquinolinyl]methyl]-3-ethenyl-3,4-dihydro-2-[(2,3,4,6-tetra-

O-acetyl- β -D-glucopyranosyl)oxy]-, methyl ester, [2S-[2 α , 3 β , 4 β (S*)]]- (9CI) (CA INDEX NAME)

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IT 122587-80-8P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of (Erratum)) RN 122587-80-8 CAPLUS CN 2H-Pyran-5-carboxylic acid, 4-[[2-acetyl-8-(acetyloxy)-1,2,3,4-tetrahydro-7-methoxy-1-isoquinolinyl]methyl]-3-ethenyl-3,4-dihydro-2-[(2,3,4,6-tetra-0-acetyl-<math>\beta-D-glucopyranosyl)oxy]-, methyl ester, [2S-[2\alpha,3\beta,4\beta(S*)]]- (9CI) (CA INDEX NAME)
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L16 ANSWER 24 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN
     1989:530718 CAPLUS Full-text
AN
DN
     111:130718
     Neoipecoside and 7-methylneoipecoside, new unusually-cyclized
TΙ
     tetrahydroisoquinoline-monoterpene glucosides from Cephaelis
ipecacuanha
ΑU
     Itoh, Atsuko; Tanahashi, Takao; Nagakura, Naotaka
     Kobe Women's Coll. Pharm., Kobe, 658, Japan
CS
     Chemical & Pharmaceutical Bulletin (1989), 37(4), 1137-9
so
     CODEN: CPBTAL; ISSN: 0009-2363
\mathbf{DT}
     Journal
     English
LA
     122587-78-4P, Neoipecoside hexaacetate
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT
     (Reactant or reagent)
        (preparation and deacetylation of)
RN
     122587-78-4 CAPLUS
     2H-Pyran-5-carboxylic acid, 4-[[2-acetyl-7,8-bis(acetyloxy)-1,2,3,4-
CN
     tetrahydro-1-isoquinolinyl]methyl]-3-ethenyl-3,4-dihydro-2-[(2,3,4,6-
tetra-
     O-acetyl-\beta-D-glucopyranosyl)oxy]-, methyl ester, [2S-
     [2\alpha, 3\beta, 4\beta(S^*)] (9CI) (CA INDEX NAME)
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L16 ANSWER 25 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN 1989:169041 CAPLUS Full-text AN DN 110:169041 Mammalian alkaloids: O-methylation of (S)- and (R)-ΤI dideoxynorlaudanosoline-1-carboxylic acid by catechol Omethyltransferase and identification of a yellow pigment obtained at physiological pH Rozwadowska, Maria Danuta; Chrzanowska, Maria; Brossi, Arnold; ΑU Creveling, Cyrus R.; Bembenek, Michael E.; Abell, Creed W. CS Lab. Anal. Chem., NIDDK, Bethesda, MD, 20892, USA so Helvetica Chimica Acta (1988), 71(7), 1598-607 CODEN: HCACAV; ISSN: 0018-019X Journal DΤ English LΑ os CASREACT 110:169041 IT 119995-28-7P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

119995-28-7 CAPLUS RN 6,7-Isoquinolinediol, 2-acetyl-1,2,3,4-tetrahydro-1-(phenylmethyl)-, CN diacetate (ester) (9CI) (CA INDEX NAME)

L16 ANSWER 26 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN1989:74990 CAPLUS Full-text

110:74990 DN

On the selectivity of O-demethylation of tetramethoxylated ΤI 1,2-diarylethylamides

ΑU Villa, M. J.; Lete, E.; Dominguez, E.

Fac. Cienc., Univ. Pais Vasco, Bilbao, 48080, Spain CS

SO Chemica Scripta (1988), 28(2), 145-8 CODEN: CSRPB9; ISSN: 0004-2056

DTJournal

English LA

CASREACT 110:74990 os

ΙT 118647-44-2P 118647-45-3P 118647-46-4P

118647-47-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN118647-44-2 CAPLUS

Acetamide, N-[2-[5-(acetyloxy)-2-bromo-4-methoxypheny1]-1-[3-methoxypheny1]CN

(acetyloxy)-4-

methoxyphenyl]ethyl]-N-formyl- (9CI) (CA INDEX NAME)

118647-45-3 CAPLUS RN

Acetamide, N-[2-[5-(acetyloxy)-2-bromo-4-methoxyphenyl]-1-[4-kg]CN (acetyloxy)-3-

methoxyphenyl]ethyl]-N-formyl- (9CI) (CA INDEX NAME)

118647-46-4 CAPLUS RN

Acetamide, N-[2-[4-(acetyloxy)-2-bromo-5-methoxyphenyl]-1-[3-CN

methoxyphenyl]ethyl]-N-formyl- (9CI) (CA INDEX NAME)

RN 118647-47-5 CAPLUS
CN Acetamide, N-[2-[4-(acetyloxy)-2-bromo-5-methoxyphenyl]-1-[4-(acetyloxy)-3methoxyphenyl]ethyl]-N-formyl- (9CI) (CA INDEX NAME)

L16 ANSWER 27 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1988:504068 CAPLUS Full-text

DN 109:104068

TI Studies on intestinal lymphatic absorption of drugs. I. Lymphatic absorption of alkyl ester derivatives and α -monoglyceride derivatives of drugs

AU - Sugihara, Juko; Furuuchi, Satoshi; Nakano, Kouzaburo; Harigaya, Shoichi

CS Biol. Res. Lab., Tanabe Seiyaku Co. Ltd., Toda, 335, Japan

SO Journal of Pharmacobio-Dynamics (1988), 11(5), 369-76 CODEN: JOPHDQ; ISSN: 0386-846X

DT Journal

LA English

IT 116048-70-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of radiolabeled and intestinal lymphatic absorption

of)

RN 116048-70-5 CAPLUS

CN Butanoic acid, 1,2,3,4-tetrahydro-1-[(3,4,5-trimethoxyphenyl)methyl]-6,7-

isoquinolinediyl ester, hydrochloride, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

HC1

L16 ANSWER 28 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

1988:406430 CAPLUS Full-text AN

109:6430 DN

TI Preparation of optically pure N-acyltetrahydroisoquinolines as pharmaceutical intermediates

IN Noyori, Ryoji; Kitamura, Masato; Takaya, Hidemasa; Kumobayashi, Hidenori;

Akutagawa, Susumu

Takasago Perfumery Co., Ltd., Japan PA

so Eur. Pat. Appl., 12 pp.

CODEN: EPXXDW

DTPatent

LA English

FAN.CNT 1

IAW. CNI I								
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE			
Ρ.	I EP 245960	A2	19871119	EP 1987-303217	19870413			
	EP 245960	A3	19881221					
	EP 245960	B1	19920729					
	R: CH, DE,	FR, GB	, LI, NL					
	JP 62265266	A2	19871118	JP 1986-108889	19860513			
	JP 03068022	B4	19911025					
	US 4851537	Α	19890725	US 1987-38571	19870415			
PI	RAI JP 1986-108889		19860513					
05	CASREACT 109:64	CASREACT 109:6430						
ľ	T 104621-45-6P							
				(

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as pharmaceutical intermediate)

104621-45-6 CAPLUS

7-Isoquinolinol, 2-acetyl-1-[[3-(acetyloxy)-4-methoxyphenyl]methyl]-1,2,3,4-tetrahydro-6-methoxy-, acetate (ester), (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L16 ANSWER 29 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1988:112803 CAPLUS Full-text

DN 108:112803

TI Synthesis of (\pm) -roemecarine and (\pm) -epiroemecarine. Revised stereostructure for (+)-roemecarine

AU Hoshino, Osamu; Itoh, Katsuhiko; Umezawa, Bunsuke; Akita, Hiroyuki; Oishi,

Takeshi

CS Fac. Pharm. Sci., Sci. Univ. Tokyo, Tokyo, 162, Japan

SO Heterocycles (1987), 26(8), 2099-100

CODEN: HTCYAM; ISSN: 0385-5414

DT Journal

LA English

OS CASREACT 108:112803

IT 96012-67-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 96012-67-8 CAPLUS

CN 4,6-Isoquinolinediol, 1-[(3,4-dimethoxyphenyl)methyl]-1,2,3,4-tetrahydro-7-

methoxy-2-methyl-, diacetate (ester), trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L16 ANSWER 30 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1987:156744 CAPLUS Full-text

DN 106:156744

TI Studies on tetrahydroisoquinolines. XXVI. A biomimetic synthesis of 5-oxygenated 1,2,3,4-tetrahydroisoquinolines

AU Hara, Hiroshi; Tsunashima, Akira; Shinoki, Hiroshi; Akiba, Toshifumi; Hoshino, Osamu; Umezawa, Bunsuke

CS Fac. Pharm. Sci., Sci. Univ. Tokyo, Tokyo, 162, Japan

SO Chemical & Pharmaceutical Bulletin (1986), 34(1), 66-70

CODEN: CPBTAL; ISSN: 0009-2363 DΤ Journal LA English os CASREACT 106:156744 ΙT 81451-72-1P 107503-19-5P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and hydrolysis-methylation of) RN81451-72-1 CAPLUS 5,6-Isoquinolinediol, 1,2,3,4-tetrahydro-7-methoxy-1-[(4methoxyphenyl)methyl]-2-methyl-, diacetate (ester) (9CI) (CA INDEX NAME)

RN 107503-19-5 CAPLUS
CN 5,6-Isoquinolinediol, 1,2,3,4-tetrahydro-7-methoxy-2-methyl-1(phenylmethyl)-, diacetate (ester) (9CI) (CA INDEX NAME)

L16 ANSWER 31 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN 1987:153047 CAPLUS Full-text DN 106:153047 Alkaloids of the Annonaceae. Part 67. Luxandrine, a quaternary benzylisoquinoline from Pseudoxandra sclerocarpa ΑU Cortes, Diego; Wannigama, G. Percy; Saez, Jairo; Cave, Andre CS Lab. Pharmacogn., Fac. Pharm., Chatenay-Malabry, 92296, Fr. Phytochemistry (1986), 25(11), 2693-5 SO CODEN: PYTCAS; ISSN: 0031-9422 \mathbf{DT} Journal LA English ΙT 107584-93-0P, O,O-Diacetylluxandrine chloride RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) 107584-93-0 CAPLUS RN CN Isoquinolinium, 6,7-bis(acetyloxy)-1,2,3,4-tetrahydro-1-[(4methoxyphenyl)methyl]-2,2-dimethyl-, chloride, (R)- (9CI) (CA INDEX

NAME)

Absolute stereochemistry.

Cl -

L16 ANSWER 32 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1987:3059 CAPLUS Full-text

DN 106:3059

TI Imbricatine, an unusual benzyltetrahydroisoquinoline alkaloid isolated from the starfish Dermasterias imbricata

AU Pathirana, Charles; Andersen, Raymond J.

CS Dep. Chem., Univ. British Columbia, Vancouver, BC, V6T 1W5, Can.

SO Journal of the American Chemical Society (1986), 108(26), 8288-9 CODEN: JACSAT; ISSN: 0002-7863

DT Journal

LA English

IT 105372-71-2P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and mass spectrum of)

RN 105372-71-2 CAPLUS

CN 3-Isoquinolinecarboxylic acid, 2-acetyl-5-[[5-[2-(acetylamino)-3-methoxy-3-

oxopropyl]-1-methyl-1H-imidazol-4-yl]thio]-6,8-bis(acetyloxy)-1-[[4-(acetyloxy)phenyl]methyl]-1,2,3,4-tetrahydro-, methyl ester, [1R-[1 α ,3 α ,5(S*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L16 ANSWER 33 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN AN1987:2899 CAPLUS Full-text DN 106:2899 Isolation and identification of N-nororientaline from Erythrina TI herbacea Linn Saqib, Qazi Najmus; Usmanghani, K.; Ahmad, V. U. ΑU Dep. Pharm., Gomal Univ., Dera Ismail Khan, Pak. CS Journal of Pharmacy (University of Karachi) (1985), 4(1), 39-42 SO CODEN: JPUKDX; ISSN: 0257-3865 DTJournal English LA IT 105701-93-7P, N-Nororientaline triacetate RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) 105701-93-7 CAPLUS RN 7-Isoquinolinol, 2-acetyl-1-[[4-(acetyloxy)-3-methoxyphenyl]methyl]-CN 1,2,3,4-tetrahydro-6-methoxy-, acetate (ester), (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L16 ANSWER 34 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN 1986:591459 CAPLUS Full-text AN DN 105:191459 Asymmetric synthesis of isoquinoline alkaloids by homogeneous catalysis Noyori, Ryoji; Ohta, Masako; Hsiao, Yi; Kitamura, Masato; Ohta, ΑU Tetsuo; Takaya, Hidemasa CS Dep. Chem., Nagoya Univ., Nagoya, 464, Japan Journal of the American Chemical Society (1986), 108(22), 7117-19 SO CODEN: JACSAT; ISSN: 0002-7863 DTJournal LA English CASREACT 105:191459 OS IT 104621-46-7P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and deacetylation of) RN104621-46-7 CAPLUS 7-Isoquinolinol, 2-acetyl-1-[[3-(acetyloxy)-4-methoxyphenyl]methyl]-CN 1,2,3,4-tetrahydro-6-methoxy-, acetate (ester), (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 104621-45-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 104621-45-6 CAPLUS

CN 7-Isoquinolinol, 2-acetyl-1-[[3-(acetyloxy)-4-methoxyphenyl]methyl] 1,2,3,4-tetrahydro-6-methoxy-, acetate (ester), (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L16 ANSWER 35 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1986:533730 CAPLUS Full-text

DN 105:133730

TI Syntheses and β -adrenergic agonist and antiaggregatory properties of N-substituted trimetoquinol analogues

AU Adejare, Adeboye; Miller, Duane D.; Fedyna, Joanne S.; Ahn, Chang Ho; Feller, Dennis R.

CS Coll. Pharm., Ohio State Univ., Columbus, OH, 43210, USA

SO Journal of Medicinal Chemistry (1986), 29(9), 1603-9 CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

OS CASREACT 105:133730

IT 102920-96-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

RACT

(Reactant or reagent)

(preparation and deacetylation of)

RN 102920-96-7 CAPLUS

CN 6,7-Isoquinolinediol, 1,2,3,4-tetrahydro-2-(phenylmethyl)-1-[(3,4,5-trimethoxyphenyl)methyl]-, diacetate (ester), hydrochloride (9CI) (CA INDEX NAME)

● HCl

IT 102920-97-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 102920-97-8 CAPLUS

CN 6,7-Isoquinolinediol, 1,2,3,4-tetrahydro-2-(phenylmethyl)-1-[(3,4,5-trimethoxyphenyl)methyl]-, diacetate (ester) (9CI) (CA INDEX NAME)

L16 ANSWER 36 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN 1985:166036 CAPLUS Full-text AN DN 102:166036 Studies on tetrahydroisoquinolines. XXIII. Reactions of (\pm) -7-acetoxy-7-methoxy-1-(3,4-dimethoxy- or 3,4methylenedioxybenzyl) -2-methyl-6-oxo- δ 4a, 5, 8, 8a-hexahydroisoquinoline (o-quinol acetate) ΑU Hoshino, Osamu; Ohtani, Minoru; Umezawa, Bunsuke; Iitaka, Yoichi Fac. Pharm. Sci., Sci. Univ. Tokyo, Tokyo, 162, Japan CS Chemical & Pharmaceutical Bulletin (1984), 32(12), 4873-82 CODEN: CPBTAL; ISSN: 0009-2363 DT Journal LA English CASREACT 102:166036 OS IT 96012-66-7P 96012-67-8P 96012-68-9P 96012-71-4P 96012-72-5P 96012-73-6P 96012-74-7P 96022-25-2P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) RN96012-66-7 CAPLUS CN Isoquinolinium, 4,6-bis(acetyloxy)-1-[(3,4-dimethoxyphenyl)methyl]-1,2,3,4-

(1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 96012-65-6 CMF C25 H32 N O7

Relative stereochemistry.

CM 2

CRN 14798-26-6 CMF C6 H2 N3 O7

RN 96012-67-8 CAPLUS

CN 4,6-Isoquinolinediol, 1-[(3,4-dimethoxyphenyl)methyl]-1,2,3,4-tetrahydro-7-

methoxy-2-methyl-, diacetate (ester), trans- (9CI) (CA INDEX NAME)

RN 96012-68-9 CAPLUS

CN Isoquinolinium, 4,6-bis(acetyloxy)-1-[(3,4-dimethoxyphenyl)methyl]-1,2,3,4-

tetrahydro-7-methoxy-2,2-dimethyl-, iodide, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

OI.

RN 96012-71-4 CAPLUS

CN 4,6-Isoquinolinediol, 1-(1,3-benzodioxol-5-ylmethyl)-1,2,3,4-tetrahydro-7-

methoxy-2-methyl-, diacetate (ester), cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 96012-72-5 CAPLUS

CN 4,6-Isoquinolinediol, 1-(1,3-benzodioxol-5-ylmethyl)-1,2,3,4-tetrahydro-7-

methoxy-2-methyl-, diacetate (ester), cis-, compd. with
2,4,6-trinitrophenol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 96012-71-4 CMF C23 H25 N O7



CM 2

CRN 88-89-1 CMF C6 H3 N3 O7

RN 96012-73-6 CAPLUS

CN 4,6-Isoquinolinediol, 1-(1,3-benzodioxol-5-ylmethyl)-1,2,3,4-tetrahydro-7-

methoxy-2-methyl-, diacetate (ester), trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 96012-74-7 CAPLUS

CN Isoquinolinium, 4,6-bis(acetyloxy)-1-(1,3-benzodioxol-5-ylmethyl)-1,2,3,4-

tetrahydro-7-methoxy-2,2-dimethyl-, iodide, trans- (9CI) (CA INDEX NAME)

• I -

RN 96022-25-2 CAPLUS

CN 4,6-Isoquinolinediol, 1-[(3,4-dimethoxyphenyl)methyl]-1,2,3,4-tetrahydro-7-

methoxy-2-methyl-, diacetate (ester), cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L16 ANSWER 37 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1984:175104 CAPLUS Full-text

DN 100:175104

TI Studies on tetrahydroisoquinolines. XXI. A synthesis of (±)-1-hydroxy-2-methoxyhomoproaporphine and stereochemistry of 4-oxygenated 1,2,3,4-tetrahydroisoquinolines

AU Hara, Hiroshi; Shirai, Ryuichi; Hoshino, Osamu; Umezawa, Bunsuke; Iitaka,

Yoichi

CS Fac. Pharm. Sci., Sci. Univ. Tokyo, Tokyo, 162, Japan

SO Chemical & Pharmaceutical Bulletin (1983), 31(12), 4236-46 CODEN: CPBTAL; ISSN: 0009-2363

DT Journal

LA English

IT 89758-71-4P 89758-83-8P 89758-88-3P

89758-89-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 89758-71-4 CAPLUS

CN 4,7-Isoquinolinediol, 1,2,3,4-tetrahydro-6-methoxy-1-[(4-methoxyphenyl)methyl]-2-methyl-, diacetate (ester), trans- (9CI) (CA INDEX NAME)

RN 89758-83-8 CAPLUS
CN 4,7-Isoquinolinediol, 1,2,3,4-tetrahydro-6-methoxy-1-[(4 methoxyphenyl)methyl]-2-methyl-, diacetate (ester), cis- (9CI) (CA
INDEX
 NAME)

Relative stereochemistry.

RN 89758-88-3 CAPLUS
CN Isoquinolinium, 4,7-bis(acetyloxy)-1,2,3,4-tetrahydro-6-methoxy-1-[(4-methoxyphenyl)methyl]-2,2-dimethyl-, iodide, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 89758-89-4 CAPLUS
CN Isoquinolinium, 4,7-bis(acetyloxy)-1,2,3,4-tetrahydro-6-methoxy-1-[(4-methoxyphenyl)methyl]-2,2-dimethyl-, iodide, cis- (9CI) (CA INDEX

NAME)

Relative stereochemistry.

• I-

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L16 ANSWER 38 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN
AN
     1984:139411 CAPLUS Full-text
DN
     100:139411
     Synthesis of 6'-methylated reticulines and tetrahydropapaverolines
ΤI
     Sharma, Padam N.; Rice, Kenner C.; Brossi, Arnold
ΑU
     Lab. Chem., Natl. Inst. Arthritis, Metab. Dig. Kidney Dis., Bethesda,
CS
MD,
     20205, USA
     Heterocycles (1983), 20(12), 2417-24
SO
     CODEN: HTCYAM; ISSN: 0385-5414
DΤ
     Journal
LA
     English
     89300-66-3
ΙT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (dechlorination of)
RN
     89300-66-3 CAPLUS
     2(1H)-Isoquinolinecarboxylic acid, 7-(acetyloxy)-1-[[5-(acetyloxy)-2-
CN
     (chloromethyl)-4-methoxyphenyl]methyl]-3,4-dihydro-6-methoxy-, ethyl
ester
     (9CI) (CA INDEX NAME)
```

IT 89240-92-6P 89240-93-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

RACT

(Reactant or reagent)

(preparation and dechlorination of)

RN 89240-92-6 CAPLUS

CN 2(1H)-Isoquinolinecarboxylic acid, 7-(acetyloxy)-1-[[5-(acetyloxy)-2-(chloromethyl)-4-methoxyphenyl]methyl]-3,4-dihydro-6-methoxy-, ethyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 89240-93-7 CAPLUS

CN 2(1H)-Isoquinolinecarboxylic acid, 7-(acetyloxy)-1-[[5-(acetyloxy)-2-(chloromethyl)-4-methoxyphenyl]methyl]-3,4-dihydro-6-methoxy-, ethyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 89300-67-4P 89300-68-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

RACT

(Reactant or reagent)

(preparation and hydrazinolysis of)

RN 89300-67-4 CAPLUS

CN 2(1H)-Isoquinolinecarboxylic acid, 7-(acetyloxy)-1-[[5-(acetyloxy)-4-methoxy-2-methylphenyl]methyl]-3,4-dihydro-6-methoxy-, ethyl ester,

(S)-

(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 89300-68-5 CAPLUS

CN 2(1H)-Isoquinolinecarboxylic acid, 7-(acetyloxy)-1-[[5-(acetyloxy)-4-methoxy-2-methylphenyl]methyl]-3,4-dihydro-6-methoxy-, ethyl ester,

(R) -

(9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 89240-94-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

RACT

(Reactant or reagent)

(preparation, reduction, and hydrazinolysis of)

RN 89240-94-8 CAPLUS

CN 2(1H)-Isoquinolinecarboxylic acid, 7-(acetyloxy)-1-[[5-(acetyloxy)-4-methoxy-2-methylphenyl]methyl]-3,4-dihydro-6-methoxy-, ethyl ester

(9CI) (CA INDEX NAME)

L16 ANSWER 39 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1983:89195 CAPLUS Full-text

DN 98:89195

TI Isoquinoline derivatives

PA Fujisawa Pharmaceutical Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 26 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

19810220 PRAI JP 1981-24812 CASREACT 98:89195 OS 84641-18-9P 84641-20-3P 84641-35-0P IT 84641-41-8P 84641-42-9P 84641-43-0P RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (preparation and antiulcer activity of) 84641-18-9 CAPLUS RN2(1H)-Isoquinolinecarboxylic acid, 6,7-bis(2,2-dimethyl-1-oxopropoxy)-CN 3,4dihydro-1-[[(1-methyl-1H-tetrazol-5-yl)amino]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 84641-20-3 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, 1,2,3,4-tetrahydro-1-[[(1-methyl-1H-tetrazol-5-yl)amino]methyl]-6,7-isoquinolinediyl ester, (2E)-2-butenedioate (2:1) (9CI) (CA INDEX NAME)

CM 1

CRN 84641-19-0 CMF C22 H32 N6 O4

CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

HO2C E CO2H

RN 84641-35-0 CAPLUS

CN 6,7-Isoquinolinediol, 2-[[4-(aminomethyl)cyclohexyl]carbonyl]-1,2,3,4-tetrahydro-1-[[(1-methyl-1H-tetrazol-5-yl)amino]methyl]-, 7-acetate (9CI)

(CA INDEX NAME)

RN 84641-41-8 CAPLUS

CN 2(1H)-Isoquinolinecarboxylic acid, 6-(2,2-dimethyl-1-oxopropoxy)-3,4-dihydro-1-[[(1-methyl-1H-tetrazol-5-yl)amino]methyl]-, phenylmethyl ester

(9CI) (CA INDEX NAME)

$$\begin{array}{c} N = N \\ N = N \\ NH \\ CH_2 \\ C = O = CH_2 = Ph \end{array}$$

RN 84641-42-9 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, 1,2,3,4-tetrahydro-1-[[(1-methyl-1H-tetrazol-5-yl)amino]methyl]-6-isoquinolinyl ester (9CI) (CA INDEX NAME)

RN 84641-43-0 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, 1,2,3,4-tetrahydro-1-[[(1-methyl-1H-tetrazol-5-yl)amino]methyl]-6-isoquinolinyl ester, ethanedioate (2:1) (9CI) (CA INDEX NAME)

CM 1

CRN 84641-42-9 CMF C17 H24 N6 O2

$$\begin{array}{c}
N = N \\
NH \\
H_2 \\
NH \\
H_3 \\
H_4 \\
H_5 \\
H_6 \\
H_7 \\
H_8 \\
H_8 \\
H_9 \\
H_9$$

CM 2

CRN 144-62-7 CMF C2 H2 O4

HO_N_O_H

L16 ANSWER 40 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1983:34820 CAPLUS Full-text

DN 98:34820

TI Synthesis of benzo[5,6]cyclohept[1,2,3,ij]isoquinolines as rigid congeners

of tetrahydropapaveroline

AU Sharma, Padam N.; Rice, Kenner C.; Brossi, Arnold

CS Lab. Chem., Natl. Inst. Arthritis, Diabetes, Dig. Kidney Dis., Bethesda,

MD, 20205, USA

SO Heterocycles (1982), 19(10), 1895-901

CODEN: HTCYAM; ISSN: 0385-5414 DT Journal English LA IT 83607-55-0P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and cyclization of) RN 83607-55-0 CAPLUS CN 2(1H)-Isoquinolinecarboxylic acid, 6-(acetyloxy)-1-[[4-(acetyloxy)-2-(chloromethy1)-5-methoxypheny1]methy1]-3,4-dihydro-7-methoxy-, ethy1 ester (9CI) (CA INDEX NAME)

L16 ANSWER 41 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN ΑN 1982:162995 CAPLUS Full-text DN 96:162995 A biomimetic synthesis of (±)-tetrahydrotakatonine, ΤI (\pm) -O-methylgigantine, and tehaunine ΑU Hara, Hirohi; Tsunashima, Akira; Shinoki, Hiroshi; Hoshino, Osamu; Umezawa, Bunsuke CS Fac. Pharm. Sci., Sci. Univ. Tokyo, Tokyo, 162, Japan Heterocycles (1982), 17 (Spec. Issue), 293-6 SO CODEN: HTCYAM; ISSN: 0385-5414 DT Journal LΑ English IT 81451-72-1P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and hydrolysis of) RN 81451-72-1 CAPLUS 5,6-Isoquinolinediol, 1,2,3,4-tetrahydro-7-methoxy-1-[(4methoxyphenyl)methyl]-2-methyl-, diacetate (ester) (9CI) (CA INDEX NAME)

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L16 ANSWER 42 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN
AN
     1982:6609 CAPLUS Full-text
DN
     96:6609
ΤI
     1,2,3,4-Tetrahydroisoquinoline derivatives
    Kishimoto, Teiji; Kochi, Hiromu; Kaneda, Yoshiyuki
IN
PA
     Fujisawa Pharmaceutical Co., Ltd., Japan
     U.S., 16 pp. Cont. of U.S. Ser. No. 695,975, abandoned.
SO
     CODEN: USXXAM
DT
     Patent
     English
LA
FAN.CNT 2
                      KIND DATE
                                           APPLICATION NO.
     PATENT NO.
                                                            DATE
                                           _____
                                                            -----
ΡI
    US 4292320
                       Α
                            19810929
                                           US 1979-67393
                                                            19790817
     JP 50035174
                       A2
                            19750403
                                           JP 1973-85987
                                                            19730730
     JP 57034275
                       В4
                            19820722
    US 3978063
                            19760831
                                           US 1974-489993
                                                            19740719
                       Α
                                           CH 1977-16303
    CH 615162
                                                            19771230
                       Α
                            19800115
                            19801015
                                           CH 1977-16304
                                                            19771230
    CH 619695
                       Α
                                           US 1980-201997
                                                            19801029
    US 4370332
                            19830125
                       Α
PRAI JP 1973-85987
                            19730730
    US 1974-489993
                            19740719
     US 1976-695975
                            19760614
     JP 1973-4882004
                            19730720
     CH 1974-9936
                            19740717
     US 1979-67393
                            19790817
os
     CASREACT 96:6609
     80128-82-1P 80128-84-3P 80128-86-5P
     80128-89-8P 80128-91-2P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT
     (Reactant or reagent)
        (preparation and deblocking of)
RN
     80128-82-1 CAPLUS
     2(1H)-Isoquinolinecarboxylic acid, 6,7-bis(acetyloxy)-3,4-dihydro-1-
CN
[(2-
     thienylthio)methyl]-, 2,2,2-trichloroethyl ester (9CI) (CA INDEX
NAME)
```

RN 80128-84-3 CAPLUS

CN 2(1H)-Isoquinolinecarboxylic acid, 6,7-bis(acetyloxy)-1-[(2-benzothiazolylthio)methyl]-3,4-dihydro-, 2,2,2-trichloroethyl ester (9CI)

(CA INDEX NAME)

RN 80128-86-5 CAPLUS

CN 2(1H)-Isoquinolinecarboxylic acid, 6,7-bis(acetyloxy)-3,4-dihydro-1-[[(5-

methyl-1,3,4-thiadiazol-2-yl)thio]methyl]-, 2,2,2-trichloroethyl ester
(9CI) (CA INDEX NAME)

RN 80128-89-8 CAPLUS

CN 2(1H)-Isoquinolinecarboxylic acid, 6,7-bis(acetyloxy)-3,4-dihydro-1-[[(1-

methyl-1H-tetrazol-5-yl)thio]methyl]-, 2,2,2-trichloroethyl ester (9CI)

(CA INDEX NAME)

$$\begin{array}{c} N = N \\ N = N \\$$

RN 80128-91-2 CAPLUS

CN 2(1H)-Isoquinolinecarboxylic acid, 3,4-dihydro-6,7-bis(2-methyl-1-oxopropoxy)-1-[[(1-methyl-1H-tetrazol-5-yl)thio]methyl]-, 2,2,2-trichloroethyl ester (9CI) (CA INDEX NAME)

IT 80128-93-4P 80128-95-6P 80128-97-8P 80129-00-6P 80129-09-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 80128-93-4 CAPLUS

CN 6,7-Isoquinolinediol, 1,2,3,4-tetrahydro-1-[(2-thienylthio)methyl]-, diacetate (ester), (2E)-2-butenedioate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 80128-92-3 CMF C18 H19 N O4 S2

CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

RN 80128-95-6 CAPLUS

CN 6,7-Isoquinolinediol, 1,2,3,4-tetrahydro-1-[[(1-methyl-1H-tetrazol-5-yl)thio]methyl]-, diacetate (ester), (2E)-2-butenedioate (salt) (9CI)

(CA

INDEX NAME)

CM 1

CRN 80128-94-5 CMF C16 H19 N5 O4 S

N— N

CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

RN 80128-97-8 CAPLUS

CN 6,7-Isoquinolinediol, 1-[(2-benzothiazolylthio)methyl]-1,2,3,4-tetrahydro-

, diacetate (ester), (2E)-2-butenedioate (2:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 80128-96-7

CMF C21 H20 N2 O4 S2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

RN 80129-00-6 CAPLUS

CN 6,7-Isoquinolinediol, 1,2,3,4-tetrahydro-1-[[(5-methyl-1,3,4-thiadiazol-2-

yl)thio]methyl]-, diacetate (ester), (2R, 3R)-2, 3-dihydroxybutanedioate (2:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 80128-99-0

CMF C17 H19 N3 O4 S2

CM 2

CRN 87-69-4 CMF C4 H6 O6

Absolute stereochemistry.

RN 80129-09-5 CAPLUS
CN Propanoic acid, 2-methyl-, 1,2,3,4-tetrahydro-1-[[(1-methyl-1H-tetrazol-5yl)thio]methyl]-6,7-isoquinolinediyl ester, (2E)-2-butenedioate (9CI)
(CA
INDEX NAME)

CM 1

CRN 80129-08-4

CMF C20 H27 N5 O4 S

CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

L16 ANSWER 43 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN 1981:565576 CAPLUS Full-text ΑN 95:165576 DN Alkaloids and olefinic acids from Cryptocarya amygdalina ΤI Borthakur, N.; Mahanta, P. K.; Rastogi, R. C. Reg. Res. Lab., Assam, 785006, India ΑU CS Phytochemistry (Elsevier) (1981), 20(3), 501-4 SO CODEN: PYTCAS; ISSN: 0031-9422 DΤ Journal English LΑ 78405-24-0P ΙT RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 78405-24-0 CAPLUS

CN 7-Isoquinolinol, 1-[[4-(acetyloxy)-3-methoxyphenyl]methyl]-1,2,3,4-tetrahydro-6-methoxy-2-methyl-, acetate (ester), (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L16 ANSWER 44 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1981:550373 CAPLUS Full-text

DN 95:150373

TI Studies on 1,2,3,4-tetrahydroisoquinoline derivatives. I. Syntheses

and

 $\beta\text{-adrenoceptor}$ activities of positional isomers of trimetoquinol with respect to its 6,7-dihydroxyl groups

AU Yamada, Koichiro; Ikezaki, Muneyoshi; Umino, Norihide; Ohtsuka, Hisao; Itoh, Nobuo; Ikezawa, Katsuo; Kiyomoto, Akio; Iwakuma, Takeo

CS Res. Lab., Tanabe Seiyaku, Co., Ltd., Saitama, 335, Japan

SO Chemical & Pharmaceutical Bulletin (1981), 29(3), 744-53 CODEN: CPBTAL; ISSN: 0009-2363

DT Journal

LA English

OS CASREACT 95:150373

IT 61831-77-4P 64728-80-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

RACT

(Reactant or reagent)

(preparation and hydrogenolysis of)

RN 61831-77-4 CAPLUS

CN 7,8-Isoquinolinediol, 1-[(3,4,5-trimethoxyphenyl)methyl]-, diacetate
 (ester) (9CI) (CA INDEX NAME)

RN 64728-80-9 CAPLUS

CN 5,7-Isoquinolinediol, 1-[(3,4,5-trimethoxyphenyl)methyl]-, diacetate
 (ester), hydrochloride (9CI) (CA INDEX NAME)

● HCl

IT 60095-77-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 60095-77-4 CAPLUS

CN 5,7-Isoquinolinediol, 1-[(3,4,5-trimethoxyphenyl)methyl]-, diacetate (ester) (9CI) (CA INDEX NAME)

L16 ANSWER 45 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1981:171027 CAPLUS Full-text

DN 94:171027

TI Isolation of higenamine from Annona squamosa; significance of adsorbent

macromolecular resins in extractive plant chemistry

- AU Leboeuf, Michel; Cave, Andre; Touche, Andre; Provost, Jean; Forgacs, Pierre
- CS Lab. Pharmacog., Fac. Pharm., Chatenay-Malabry, F 92290, Fr.
- SO Journal of Natural Products (1981), 44(1), 53-60 CODEN: JNPRDF; ISSN: 0163-3864
- DT Journal
- LA French
- IT 60941-91-5P 77354-35-9P 77354-36-0P

77354-37-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 60941-91-5 CAPLUS

CN 6,7-Isoquinolinediol, 1-[[4-(acetyloxy)phenyl]methyl]-1,2,3,4-tetrahydro-,

diacetate (ester) (9CI) (CA INDEX NAME)

RN 77354-35-9 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, 1-[[4-(2,2-dimethyl-1-oxopropoxy)phenyl]methyl]-1,2,3,4-tetrahydro-6,7-isoquinolinediylester

(9CI) (CA INDEX NAME)

RN 77354-36-0 CAPLUS

CN Butanoic acid, 1,2,3,4-tetrahydro-1-[[4-(1-oxobutoxy)phenyl]methyl]-6,7-

isoquinolinediyl ester (9CI) (CA INDEX NAME)

RN 77354-37-1 CAPLUS

Propanoic acid, 2-methyl-, 1,2,3,4-tetrahydro-1-[[4-(2-methyl-1-oxopropoxy)phenyl]methyl]-6,7-isoquinolinediyl ester (9CI) (CA INDEX NAME)

L16 ANSWER 46 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1980:198704 CAPLUS Full-text

DN 92:198704

TI Synthesis and proton and carbon-13 NMR spectroscopic studies of monoterpenoid isoquinolines

AU Hoefle, Gerhard; Nagakura, Naotaka; Zenk, Meinhart H.

CS Ges. Biotechnol. Forsch. m.b.H., Braunschweig, D-3300, Fed. Rep. Ger.

SO Chemische Berichte (1980), 113(2), 566-76 CODEN: CHBEAM; ISSN: 0009-2940

DT Journal

LA German

IT 21104-39-2P 21104-40-5P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and NMR of)

RN 21104-39-2 CAPLUS

CN 2H-Pyran-5-carboxylic acid, 4-[[2-acetyl-6,7-bis(acetyloxy)-1,2,3,4-tetrahydro-1-isoquinolinyl]methyl]-3-ethenyl-3,4-dihydro-2-[(2,3,4,6-tetra-

O-acetyl- β -D-glucopyranosyl)oxy]-, methyl ester, [2S-[2 α , 3 β , 4 β (S*)]]- (9CI) (CA INDEX NAME)

RN 21104-40-5 CAPLUS

CN 2H-Pyran-5-carboxylic acid, 4-[[2-acetyl-6,7-bis(acetyloxy)-1,2,3,4-tetrahydro-1-isoquinolinyl]methyl]-3-ethenyl-3,4-dihydro-2-[(2,3,4,6-tetra-

O-acetyl- β -D-glucopyranosyl)oxy]-, methyl ester, [2S-[2 α , 3 β , 4 β (R*)]]- (9CI) (CA INDEX NAME)

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L16 ANSWER 47 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN
     1979:100170 CAPLUS Full-text
AN
     90:100170
DN
     Deacetylisoipecoside: the key intermediate in the biosynthesis of the
ΤI
     alkaloids cephaeline and emetine
     Nagakura, Naotaka; Hoefle, Gerhard; Zenk, Meinhart H.
ΑU
     Lehrstuhl Pfanzenphysiol., Ruhr Univ. Bochum, Bochum, Fed. Rep. Ger.
CS
     Journal of the Chemical Society, Chemical Communications (1978), (20),
so
     896-8
     CODEN: JCCCAT; ISSN: 0022-4936
DT
     Journal
     English
LA
ΙT
     21104-39-2
     RL: BIOL (Biological study)
        (CD of)
RN
     21104-39-2 CAPLUS
     2H-Pyran-5-carboxylic acid, 4-[[2-acetyl-6,7-bis(acetyloxy)-1,2,3,4-
CN
     tetrahydro-1-isoquinolinyl]methyl]-3-ethenyl-3,4-dihydro-2-[(2,3,4,6-
tetra-
     O-acetyl-\beta-D-glucopyranosyl)oxy]-, methyl ester, [2S-
     [2\alpha, 3\beta, 4\beta(s^*)] (9CI) (CA INDEX NAME)
```

AcO OAC OAC OAC
$$AcO$$
 CH2 C CH2 C AcO AcO AcO AcO AcO AcO AcO AcO AcO AcO AcO

```
L16 ANSWER 48 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1978:439396 CAPLUS <u>Full-text</u>
DN 89:39396
TI The alkaloids of Thalictrum dioicum L
AU Shamma, Maurice; Rothenberg, Alan S.
```

AU Shamma, Maurice; Rothenberg, Alan S.
CS Dep. Chem., Pennsylvania State Univ., University Park, PA, USA

Lloydia (1978), 41(2), 169-78 CODEN: LLOYA2; ISSN: 0024-5461

DΤ Journal

LA English

32490-10-1P IT

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

32490-10-1 CAPLUS RN

7-Isoquinolinol, 1-[[4-(acetyloxy)phenyl]methyl]-1,2,3,4-tetrahydro-6-CNmethoxy-2-methyl-, acetate (ester), (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L16 ANSWER 49 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1977:601342 CAPLUS Full-text

DN 87:201342

TI Tetrahydroisoquinolines

Ikezaki, Munekatsu; Irie, Kunihiko; Unno, Tokuei; Ikezawa, Ichiro; IN Sato,

Masanori

Tanabe Seiyaku Co., Ltd., Japan PA

Jpn. Kokai Tokkyo Koho, 5 pp. SO

CODEN: JKXXAF

DΤ Patent

LAJapanese

FAN.	CNT I				
	PATENT NO.	NO. KIND DATE	DATE	APPLICATION NO.	DATE
PI	JP 52102281	A2	19770827	JP 1976-19593	19760224
	JP 56019871	B4	19810509		
PRAI	JP 1976-19593		19760224		
IT	60095-77-4P				

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and conversion to hydrochloride)

RN 60095-77-4 CAPLUS

5,7-Isoquinolinediol, 1-[(3,4,5-trimethoxyphenyl)methyl]-, diacetate CN (ester) (9CI) (CA INDEX NAME)

IT 64728-80-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

RACT

(Reactant or reagent)

(preparation and hydrogenation of)

RN 64728-80-9 CAPLUS

CN 5,7-Isoquinolinediol, 1-[(3,4,5-trimethoxyphenyl)methyl]-, diacetate (ester), hydrochloride (9CI) (CA INDEX NAME)

● HCl

L16 ANSWER 50 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1977:121339 CAPLUS Full-text

DN 86:121339

TI Tetrahydroisoquinolines

IN Kishimoto, Teiji; Kouchi, Hiromu; Kaneda, Yoshiyuki

PA Fujisawa Pharmaceutical Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 5 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN. CNT 1

EMM.	PATENT NO.	KIND DATE APPLICAT		APPLICATION NO.	DATE	
ΡI	JP 51086477	A2	19760729	JP 1975-8187	19750117	
	JP 58017472	B4	19830407			
PRAI	JP 1975-8187		19750117			
~~	GRODERGE 0C.1010	2.0				

OS CASREACT 86:121339

IT 61809-61-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(deprotection of)

RN 61809-61-8 CAPLUS

6,7-Isoquinolinediol, 2-acetyl-1,2,3,4-tetrahydro-1-[[(1-methyl-1H-CN tetrazol-5-yl)thio]methyl]-, diacetate (ester) (9CI) (CA INDEX NAME)

L16 ANSWER 51 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN1977:106409 CAPLUS Full-text

DN 86:106409

Tetrahydroisoquinolines

Ikezaki, Muneyoshu; Irie, Kunihiko; Umino, Norihide; Ikezawa, Kazuo; Satoh, Masanori

Tanabe Seiyaku Co., Ltd., Japan PA

Jpn. Kokai Tokkyo Koho, 11 pp. so

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

APPLICATION NO. DATE PATENT NO. KIND DATE JP 51070774 JP 1974-140294 19741205 19760618 PΙ A2 19741205

PRAI JP 1974-140294

61831-77-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

RACT

(Reactant or reagent)

(preparation and hydrogenation of)

RN 61831-77-4 CAPLUS

7,8-Isoquinolinediol, 1-[(3,4,5-trimethoxyphenyl)methyl]-, diacetate CN (ester) (9CI) (CA INDEX NAME)

61831-78-5P TΤ

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

RACT

(Reactant or reagent)
 (preparation and hydrolysis of)

RN 61831-78-5 CAPLUS

CN 7,8-Isoquinolinediol, 1-[(3,4,5-trimethoxyphenyl)methyl]-, diacetate (ester), hydrochloride (9CI) (CA INDEX NAME)

● HCl

L16 ANSWER 52 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1977:89826 CAPLUS Full-text

DN 86:89826

TI Tetrahydroisoquinolines

IN Kishimoto, Teiji; Kouchi, Hiromu; Kaneda, Yoshiyuki

PA Fujisawa Pharmaceutical Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 4 pp. CODEN: JKXXAF

Patent

LA Japanese

FAN.CNT 1

DT

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 51086478 PRAI JP 1975-8188	A2	19760729 19750117	JP 1975-8188	19750117

IT 61809-61-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 61809-61-8 CAPLUS

CN 6,7-Isoquinolinediol, 2-acetyl-1,2,3,4-tetrahydro-1-[[(1-methyl-1H-tetrazol-5-yl)thio]methyl]-, diacetate (ester) (9CI) (CA INDEX NAME)

$$\begin{array}{c} N = N \\ N = N \\$$

L16 ANSWER 53 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

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1977:72465 CAPLUS Full-text
AN
    86:72465
DN
ΤI
    Tetrahydroisoquinolines
    Ikezaki, Muneyoshi; Irie, Kunihiko; Umino, Norihide; Ikezawa, Kazuo;
IN
    Satoh, Masanori
    Tanabe Seiyaku Co., Ltd., Japan
PA
    Jpn. Kokai Tokkyo Koho, 6 pp.
SO
    CODEN: JKXXAF
DT
    Patent
LA
    Japanese
FAN.CNT 1
                                        APPLICATION NO. DATE
                   KIND DATE
    PATENT NO.
    _____
                                        _____
                                        JP 1974-137166 19741127
                    A2
                          19760618
    JP 51070772
PRAI JP 1974-137166
                         19741127
    61672-56-8P
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT
    (Reactant or reagent)
       (preparation and hydrogenation of)
    61672-56-8 CAPLUS
RN
    5-Isoquinolinol, 1-[(3,4,5-trimethoxyphenyl)methyl]-, acetate (ester),
CN
    hydrochloride (9CI) (CA INDEX NAME)
```

HCl

```
L16 ANSWER 54 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN
   1976:592960 CAPLUS Full-text
AN
DN
    85:192960
ΤI
    O-Acylhigenamines
    Okamoto, Toshihiko; Kosuga, Takuo; Yokota, Masami
IN
    Hokuriku Pharmaceutical Co., Ltd., Japan
PA
SO
    Jpn. Kokai Tokkyo Koho, 3 pp.
    CODEN: JKXXAF
DT
    Patent
LA
    Japanese
FAN.CNT 1
                                       APPLICATION NO. DATE
    PATENT NO. KIND DATE
                    ----
    _____
    JP 51048677
                     A2 19760426
                                        JP 1974-121715 19741022
PΙ
PRAI JP 1974-121715
                         19741022
    60941-90-4P
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
```

RACT

(Reactant or reagent)
 (preparation and hydrogenation of)

RN 60941-90-4 CAPLUS

CN 2(1H)-Isoquinolinecarboxylic acid, 6,7-bis(acetyloxy)-1-[[4-(acetyloxy)phenyl]methyl]-3,4-dihydro-, phenylmethyl ester (9CI) (CA INDEX NAME)

IT 60941-91-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 60941-91-5 CAPLUS

CN 6,7-Isoquinolinediol, 1-[[4-(acetyloxy)phenyl]methyl]-1,2,3,4-tetrahydro-,

diacetate (ester) (9CI) (CA INDEX NAME)

L16 ANSWER 55 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1976:478022 CAPLUS Full-text

DN 85:78022

TI 5,7-Dihydroxytetrahydroisoquinoline derivatives

IN Ikezaki, Muneyoshi; Irie, Kunihiko; Umino, Norihide; Ikezawa, Katsuo; Sato, Masanori

PA Tanabe Seiyaku Co., Ltd., Japan

SO Ger. Offen., 23 pp. CODEN: GWXXBX

m D-+--+

DT Patent

LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2551924	A1	19760526	DE 1975-2551924	19751119
	DE 2551924	B2	19770526		

	JΡ	51070770	A2	19760618	JР	1974-134734	19741120
	JΡ	52047474	B4	19771202			
	DK	7504873	Α	19760521	DK	1975-4873	19751029
	DK	143197	В	19810720			
	DK	143197	С	19811123			
	GB	1487457	A	19770928		1975-44807	19751030
	US	4054659	A	19771018		1975-627259	19751030
	ΑU	7586713	A1	19770317		1975-86713	19751118
	CA	1032541	A1	19780606		1975-239977	19751118
	CS	190503	P	19790531	CS	1975-7781	19751118
	BE	835744	A1	19760316	BE	1975-6045258	
	SE	7513013	A	19760521	SE	1975-13013	19751119
	SE	424638	В	19820802			
	SE	424638	С	19821111			
	NL	7513517	A	19760524	NL	1975-13517	19751119
	NL	166469	В	19810316			
	NL	166469	С	19810817			
	FR	2291753	A1	19760618	FR	1975-35390	19751119
	FR	2291753	B1	19781110			
	HU	170648	P	19770728	HU	1975-TA1379	19751119
	CH	621341	A	19810130	CH	1975-15048	19751120
	CH	623039	Α	19810515	CH	1980-6065	19800811
PRAI	JP	1974-134734		19741120			
	CH	1975-15048		19751120			
IT	600	095-77-4P					
	RL:	RCT (Reactant); SPI	N (Synthetic pro	epai	ration); PREP	(Preparation);
RACT							
	(Re	eactant or reage	ent)				
		(preparation as	nd re	duction of)			
RN	600	095-77-4 CAPLU	S				
CN	5,7	7-Isoquinolined	iol,	1-[(3,4,5-trime	tho	kyphenyl) methy:	l]-, diacetate
	(es	ster) (9CI) (C	A IND	EX NAME)			

```
L16 ANSWER 56 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN
AN
     1975:606461 CAPLUS Full-text
DN
     83:206461
     Proaporhine and aporphine alkaloids. V. Synthesis of (+)-glaziovine
TI
by
     8,1'-ring closure of 1-benzylisoquinoline derivatives
     Casagrande, Cesare; Canonica, Luigi
ΑU
     Lab. Ric. Chim., Simes S.p.A., Milan, Italy
CS
     Journal of the Chemical Society, Perkin Transactions 1: Organic and
so
     Bio-Organic Chemistry (1972-1999) (1975), (17), 1647-52
     CODEN: JCPRB4; ISSN: 0300-922X
```

DT Journal

LA English

IT 58093-40-6P 58093-41-7P 58093-42-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 58093-40-6 CAPLUS

CN Isoquinoline, 7-(acetyloxy)-1-[[4-(acetyloxy)phenyl]methyl]-1,2,3,4-tetrahydro-6-methoxy-2-(trifluoroacetyl)- (9CI) (CA INDEX NAME)

RN 58093-41-7 CAPLUS

CN Isoquinoline, 7-(acetyloxy)-1-[[4-(acetyloxy)phenyl]methyl]-8-chloro-1,2,3,4-tetrahydro-6-methoxy-2-(trifluoroacetyl)- (9CI) (CA INDEX NAME)

RN 58093-42-8 CAPLUS

CN Isoquinoline, 4,7-bis(acetyloxy)-1-[[4-(acetyloxy)phenyl]methyl]-8-chloro-

1,2,3,4-tetrahydro-6-methoxy-2-(trifluoroacetyl)- (9CI) (CA INDEX NAME)

L16 ANSWER 57 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1975:514235 CAPLUS Full-text

DN 83:114235

TI Tetrahydroisoquinoline derivatives

IN Irie, Kunihiko; Ito, Nobuo; Sugasawa, Shigehiko; Ikezawa, Kazuo; Sato, Masanori

PA Tanabe Seiyaku Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 7 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	KIND DATE	APPLICATION NO.	DATE	
		-				
PΙ	JP 50035175	A2	19750403	JP 1973-86072	19730731	
	JP 52046232	В4	19771122			
PRA	I JP 1973-86072		19730731			

IT 56629-28-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(hydrolysis of)

RN 56629-28-8 CAPLUS

CN 7-Isoquinolinol, 1,2,3,4-tetrahydro-1-[(3,4,5-

trimethoxyphenyl)methyl]-,

acetate (ester), hydrochloride (9CI) (CA INDEX NAME)

● HCl

L16 ANSWER 58 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1975:427935 CAPLUS Full-text

DN 83:27935

TI $N-[\alpha-(3,4-Diacyloxyphenyl)-\beta-arylethyl]-carbamates$

IN Yamamura, Toshiro; Ohashi, Motoaki; Saito, Seiichi; Iwasawa, Yoshio; Harigaya, Shoichi

PA Tanabe Seiyaku Co., Ltd.

SO Jpn. Kokai Tokkyo Koho, 4 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI JP 49135955	A2	19741227	JP 1973-53352	19730514	
PRAI JP 1973-53352		19730514			

IT 56064-56-3P 56064-57-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 56064-56-3 CAPLUS

CN Carbamic acid, [1-[3,4-bis(acetyloxy)phenyl]-2-(3,4-

dimethoxyphenyl)ethyl]-

, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 56064-57-4 CAPLUS

CN Carbamic acid, [1-[3,4-bis(acetyloxy)phenyl]-2-(3,4,5-trimethoxyphenyl)ethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

L16 ANSWER 59 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1975:156025 CAPLUS Full-text

DN 82:156025

TI Tetrahydroisoquinolines. VIII. Lead tetraacetate oxidation of 1,2,3,4-tetrahydro-6-hydroxy-7-methoxy-2-methylisoquinoline and its 1-substituted derivatives

AU Hoshino, Osamu; Ohyama, Keiko; Taga, Michinori; Umezawa, Bunsuke

CS Fac. Pharm. Sci., Sci. Univ. Tokyo, Tokyo, Japan

SO Chemical & Pharmaceutical Bulletin (1974), 22(11), 2587-92 CODEN: CPBTAL; ISSN: 0009-2363

DT Journal

LA English

IT 55161-55-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 55161-55-2 CAPLUS

CN Isoquinolinium, 4,6-bis(acetyloxy)-1,2,3,4-tetrahydro-7-methoxy-2,2-dimethyl-1-(phenylmethyl)-, iodide (9CI) (CA INDEX NAME)

♠ T -

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L16 ANSWER 60 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN
    1974:569676 CAPLUS Full-text
AN
DN
    81:169676
    1-Phenethylisoquinoline alkaloids. IV. Isolation, structural
ΤI
     elucidation, and synthesis of C-homoaporphines
    Battersby, Alan R.; Bradbury, Robert B.; Herbert, Richard B.; Munro,
ΑU
    Murray H. G.; Ramage, Robert
CS
    Robert Robinson Lab., Univ. Liverpool, Liverpool, UK
     Journal of the Chemical Society, Perkin Transactions 1: Organic and
SO
    Bio-Organic Chemistry (1972-1999) (1974), (12), 1394-9
    CODEN: JCPRB4; ISSN: 0300-922X
DT
    Journal
    English
LA
    54370-10-4P
    RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
RN
     54370-10-4 CAPLUS
    7-Isoquinolinol, 1-[2-[4-(acetyloxy)-3,5-dimethoxyphenyl]ethyl]-
CN
1,2,3,4-
     tetrahydro-6-methoxy-2-methyl-, acetate (ester) (9CI) (CA INDEX NAME)
```

L16 ANSWER 61 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1974:505783 CAPLUS Full-text
DN 81:105783
TI (+-)-Glaziovine
IN Casagrande, Cesare; Canonica, Luigi
PA SIPHAR S. A.
SO Ger. Offen., 23 pp.
CODEN: GWXXBX
DT Patent

LA FAN.	German CNT 2				
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2363530	A1	19740627	DE 1973-2363530	19731220
	CH 575930	Α	19760531	CH 1972-18784	19721222
	GB 1451377	A	19760929	GB 1973-57205	19731210
	ZA 7309528	A	19741127	ZA 1973-9528	19731218
	FR 2211433	A1	19740719	FR 1973-45942	19731221
	CA 1014158	A1	19770719	CA 1973-188805	19731221
	JP 50004079	A2	19750116	JP 1974-4872	19731222
	ES 421744	A1	19760416	ES 1973-421744	19731222
PRAI	CH 1972-18784		19721222		
IT	54170-07-9P				
	RL: SPN (Synthet	ic pre	paration); PREF	(Preparation)	

(preparation of)

54170-07-9 CAPLUS RN

CN 7-Isoquinolinol, 8-bromo-1,2,3,4-tetrahydro-6-methoxy-2-methyl-1-[[4-(phenylmethoxy)phenyl]methyl]-, acetate (ester) (9CI) (CA INDEX NAME)

L16 ANSWER 62 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN1974:505313 CAPLUS Full-text

DN 81:105313

TI 6,7-Dihydroxy-1,2,3,4-tetrahydroisoquinolines

IN Kishimoto, Teiji; Kouchi, Hiromu; Kaneda, Yoshiyuki

PA Fujisawa Pharmaceutical Co., Ltd.

SO Jpn. Kokai Tokkyo Koho, 7 pp.

CODEN: JKXXAF

DTPatent

LA Japanese

FAN.	CNT	6			
	PATENT NO.		KIND	DATE	APPLICATION NO. DATE
ΡI	JР	49020187	A2	19740222	JP 1972-61961 19720620
	JΡ	55000381	B4	19800108	
	CA	990725	A1	19760608	CA 1973-173937 19730613
	CH	592629	Α	19771031	CH 1973-8900 19730619
	ES	416095	A1	19760516	ES 1973-416095 19730620
	AT	7502024	Α	19760415	AT 1975-2024 19750317
	ΑT	333762	В	19761210	
PRAI	JP	1972-61960		19720620	
	JΡ	1972-61961		19720620	
	JР	1972-61962		19720620	
	JР	1972-61963		19720620	
	JP	1972-100210		19721005	
	JР	1972-100211		19721005	

AT 1973-5381 19730619 IT 53593-12-7 53593-15-0 53593-16-1

RL: RCT (Reactant); RACT (Reactant or reagent) (hydrolysis of)

53593-12-7 CAPLUS RN

CN 6,7-Isoquinolinediol, 2-acetyl-1-[(4-chlorophenoxy)methyl]-1,2,3,4tetrahydro-, diacetate (ester) (9CI) (CA INDEX NAME)

RN 53593-15-0 CAPLUS

6,7-Isoquinolinediol, 2-acetyl-1-[(2-chloro-4-methoxyphenoxy)methyl]-CN 1,2,3,4-tetrahydro-, diacetate (ester) (9CI) (CA INDEX NAME)

RN 53593-16-1 CAPLUS

6,7-Isoquinolinediol, 2-acetyl-1-[(3,4-dichlorophenoxy)methyl]-CN 1,2,3,4-

tetrahydro-, diacetate (ester) (9CI) (CA INDEX NAME)

L16 ANSWER 63 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN 1974:96187 CAPLUS Full-text AN DN 80:96187 ΤI Simple synthesis of an isopavine alkaloid, (+)-O-methylthalisopavine and (+)-reframine ΑU Hoshino, Osamu; Tata, Michinori; Umezawa, Bunsuke CS Fac. Pharm. Sci., Sci. Univ. Tokyo, Tokyo, Japan Heterocycles (1973), 1(3-4), 223-6 so CODEN: HTCYAM; ISSN: 0385-5414 \mathbf{DT} Journal LA English IT 51724-65-3P 51724-69-7P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) RN 51724-65-3 CAPLUS CN Isoquinolinium, 4,6-bis(acetyloxy)-1-[(3,4-dimethoxyphenyl)methyl]-1,2,3,4tetrahydro-7-methoxy-2,2-dimethyl-, iodide (9CI) (CA INDEX NAME)

• I-

RN 51724-69-7 CAPLUS
CN Isoquinolinium, 4,6-bis(acetyloxy)-1-(1,3-benzodioxol-5-ylmethyl)1,2,3,4tetrahydro-7-methoxy-2,2-dimethyl-, iodide (9CI) (CA INDEX NAME)

OI.

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L16 ANSWER 64 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN
     1973:526676 CAPLUS Full-text
AN
DN
     79:126676
TТ
     Syntheses of heterocyclic compounds. DXXIII. Enzymic oxidation of
     homoorientaline with homogenized potato peelings
AU
     Kametani, T.; Mizushima, M.; Takano, S.; Fukumoto, K.
     Pharm. Inst., Tohoku Univ., Sendai, Japan
CS
     Tetrahedron (1973), 29(14), 2031-3
SO
     CODEN: TETRAB; ISSN: 0040-4020
DT
     Journal
LA
    English
     50678-01-8P
IT
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
RN
     50678-01-8 CAPLUS
     1,7-Isoquinolinediol, 1-[2-[4-(acetyloxy)-3-methoxyphenyl]ethyl]-
1,2,3,4-
     tetrahydro-6-methoxy-2-methyl-, diacetate (ester), (S)- (9CI) (CA
INDEX
    NAME)
```

Absolute stereochemistry.

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L16 ANSWER 65 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN
    1973:442719 CAPLUS Full-text
AN
DN
    79:42719
ΤI
    Intramolecular oxidative coupling of monophenolic benzylisoquinolines.
    Quinonoid oxoaporphines
ΑU
    Kupchan, S. Morris; Liepa, Andris J.
    Dep. Chem., Univ. Virginia, Charlottesville, VA, USA
    Journal of the American Chemical Society (1973), 95(12), 4062-4
    CODEN: JACSAT; ISSN: 0002-7863
    Journal
DT
LA
    English
IT
     42922-19-0P
    RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
RN
    42922-19-0 CAPLUS
    7-Isoquinolinol, 1-[(2-amino-4,5-dimethoxyphenyl)methyl]-6-methoxy-,
CN
    acetate (ester) (9CI) (CA INDEX NAME)
```

L16 ANSWER 66 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1972:488742 CAPLUS Full-text

DN 77:88742

TI Nonaromatic ring D analog of the dibenzopyrrocoline alkaloids

AU Morrison, Glenn C.; Waite, Ronald O.; Shavel, John, Jr.

CS Dep. Org. Chem., Warner-Lambert Res. Inst., Morris Plains, NJ, USA

SO Journal of Heterocyclic Chemistry (1972), 9(3), 683-5

CODEN: JHTCAD; ISSN: 0022-152X

DT Journal

LA English

IT 31804-77-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 31804-77-0 CAPLUS

CN 6-Isoquinolinol, 2-acetyl-1,2,3,4-tetrahydro-7-methoxy-1-[(4-oxo-2-cyclohexen-1-yl)methyl]-, acetate (ester) (8CI) (CA INDEX NAME)

L16 ANSWER 67 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1972:459392 CAPLUS Full-text

DN 77:59392

TI Whole-body autoradiographic studies on the distribution of radioisotopes.

 $\tt XXVIII.$ Distribution of radioactivity in mice after oral administration

of tritium labeled O-dibutyrylated trimethoquinol (BAQ-509)

AU Otsuka, Minezo; Sakuma, Mari; Sato, Yoshishige

CS Biol. Res. Lab., Tanabe Seiyaku Co. Ltd., Toda, Japan

SO Radioisotopes (1972), 21(2), 102-9

CODEN: RAISAB; ISSN: 0033-8303

DT Journal

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LA
     Japanese
IT
     37893-95-1
    RL: BPR (Biological process); BSU (Biological study, unclassified);
BIOL
     (Biological study); PROC (Process)
        (metabolism of)
RN
    37893-95-1 CAPLUS
CN
    Butanoic acid, 1,2,3,4-tetrahydro-1-[(3,4,5-trimethoxyphenyl)methyl]-
6,7-
    isoquinolinediyl ester, (2R, 3R)-2,3-dihydroxybutanedioate (1:1) (9CI)
(CA
    INDEX NAME)
    CM
         1
    CRN
         47765-22-0
    CMF C27 H35 N O7
```

CRN 87-69-4 CMF C4 H6 O6

Absolute stereochemistry.

L16 ANSWER 68 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN 1972:448280 CAPLUS <u>Full-text</u> AN Ţ DN 77:48280 ΤI Tetrahydroisoquinoline derivatives IN Watanabe, Toshiro; Hayashi, Kimiaki; Sato, Yoshinori; Iwasawa, Yoshiro PA Tanabe Seiyaku Co., Ltd. Jpn. Tokkyo Koho, 4 pp. SO CODEN: JAXXAD DT Patent LA Japanese FAN.CNT 1 PATENT NO. KIND DATE APPLICATION NO. DATE

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ΡI
    JP 47014108
                      B4 19720427
                                           JP 1969-53256
                                                            19690704
    34202-91-0P 34221-51-7P 34221-52-8P
    RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
RN
    34202-91-0 CAPLUS
CN
    Butanoic acid, 1,2,3,4-tetrahydro-1-[(3,4,5-trimethoxyphenyl)methyl]-
6,7-
    isoquinolinediyl ester, ethanedioate (1:1) (9CI) (CA INDEX NAME)
    CM
         1
    CRN 47765-22-0
    CMF C27 H35 N O7
```

CRN 144-62-7 CMF C2 H2 O4

CMF C23 H27 N O7

CRN 144-62-7 CMF C2 H2 O4

RN 34221-52-8 CAPLUS

CN Propanoic acid, 2-methyl-, 1,2,3,4-tetrahydro-1-[(3,4,5-trimethoxyphenyl)methyl]-6,7-isoquinolinediyl ester, ethanedioate (1:1)

(9CI) (CA INDEX NAME)

CM 1

CRN 34685-11-5 CMF C27 H35 N O7

CM 2

CRN 144-62-7 CMF C2 H2 O4

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L16 ANSWER 69 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN
AN
     1972:72378 CAPLUS Full-text
DN
     76:72378
TΙ
     Reaction between isatin and amines
ΑU
     Brouwer, W. G.; Craig, W. A.; Jeffreys, J. A. D.; Munro, A.
     Dep. Pure Appl. Chem., Univ. Strathclyde, Glasgow, UK
CS
     Journal of the Chemical Society, Perkin Transactions 1: Organic and
SO
     Bio-Organic Chemistry (1972-1999) (1972), (1), 124-9
     CODEN: JCPRB4; ISSN: 0300-922X
DΤ
     Journal
LA
     English
IT
     35117-99-8P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
     35117-99-8 CAPLUS
RN
CN
     6-Isoquinolinol, 1-[[3-(acetyloxy)-4-methoxyphenyl]methyl]-7-methoxy-,
     acetate (ester) (9CI) (CA INDEX NAME)
```

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L16 ANSWER 70 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN
AN
    1972:34129 CAPLUS Full-text
DN
     76:34129
ΤI
     Tetrahydroisoquinolines
IN
     Watanabe, Toshiro; Tsukamoto, Goro; Hayashi, Kimiaki; Sato, Tadanori
PA
     Tanabe Seiyaku Co., Ltd.
SO
     Jpn. Tokkyo Koho, 4 pp.
     CODEN: JAXXAD
DT
     Patent
LΑ
     Japanese
FAN.CNT 1
     PATENT NO.
                      KIND DATE
                                          APPLICATION NO. DATE
PI
     JP 46039700
                       B4
                            19711122
                                           JΡ
                                                            19690313
IT
     33300-96-8P 34685-11-5P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
RN
    33300-96-8 CAPLUS
     6,7-Isoquinolinediol, 1,2,3,4-tetrahydro-1-[(3,4,5-
     trimethoxyphenyl)methyl]-, diacetate (ester) (9CI) (CA INDEX NAME)
```

RN 34685-11-5 CAPLUS
CN Propanoic acid, 2-methyl-, 1,2,3,4-tetrahydro-1-[(3,4,5-trimethoxyphenyl)methyl]-6,7-isoquinolinediyl ester (9CI) (CA INDEX

NAME)

L16 ANSWER 71 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1972:34077 CAPLUS Full-text

DN 76:34077

TI Tetrahydroisoquinolines. I. Formation and acid-catalyzed rearrangement

of 10-acetoxy-6-methoxy-2-methyl-7-oxo- δ 5,6,8,9-hexahydroisoquinolines

AU Umezawa, Bunsuke; Hoshino, Osamu; Terayama, Yasuo; Ohyama, Keiko; Yamanashi, Yasuhiro; Inoue, Tsutomu; Toshioka, Tadashi

CS Fac. Pharm. Sci., Sci. Univ. Tokyo, Tokyo, Japan

SO Chemical & Pharmaceutical Bulletin (1971), 19(10), 2138-46 CODEN: CPBTAL; ISSN: 0009-2363

DT Journal

LA English

IT 35006-05-4P 35006-06-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 35006-05-4 CAPLUS

CN 4,7-Isoquinolinediol, 1,2,3,4-tetrahydro-6-methoxy-2-methyl-1-(phenylmethyl)-, diacetate (ester) (9CI) (CA INDEX NAME)

RN 35006-06-5 CAPLUS

CN 4,7-Isoquinolinediol, 1,2,3,4-tetrahydro-6-methoxy-2-methyl-1- (phenylmethyl)-, diacetate (ester), compd. with 2,4-dihydro-5-methyl-4-

nitro-2-(4-nitrophenyl)-3H-pyrazol-3-one (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 35006-05-4 CMF C22 H25 N O5

CM 2

CRN 550-74-3 CMF C10 H8 N4 O5

L16 ANSWER 72 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1971:488505 CAPLUS Full-text

DN 75:88505

TI Tetrahydroisoquinoline derivatives

IN Watanabe, Toshiro; Tsukamoto, Goro; Hayashi, Kimiaki; Sato, Kuninori; Iwasawa, Yoshiro

PA Tanabe Seiyaku Co., Ltd.

SO Jpn. Tokkyo Koho, 3 pp.

CODEN: JAXXAD

DT Patent

LA Japanese

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE

JP 46023389 B4 19710703 JP 19681210

IT 33300-96-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 33300-96-8 CAPLUS

CN 6,7-Isoquinolinediol, 1,2,3,4-tetrahydro-1-[(3,4,5-

trimethoxyphenyl)methyl]-, diacetate (ester) (9CI) (CA INDEX NAME)

L16 ANSWER 73 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1971:436410 CAPLUS Full-text

DN 75:36410

TI Syntheses of heterocyclic compounds. CMII. Chemical and enzymic phenol

oxidation of (R) (-)-N-methylcoclaurine and (S) (+)-reticuline

AU Kametani, Tetsuji; Fukumoto, Keiichiro; Kigasawa, Kazuo; Wakisaka, Kikuo

CS Pharm. Inst., Tohoku Univ., Sendai, Japan

SO Chemical & Pharmaceutical Bulletin (1971), 19(4), 714-17

CODEN: CPBTAL; ISSN: 0009-2363

DT Journal

LA English

IT 32490-10-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 32490-10-1 CAPLUS

CN 7-Isoquinolinol, 1-[[4-(acetyloxy)phenyl]methyl]-1,2,3,4-tetrahydro-6-methoxy-2-methyl-, acetate (ester), (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L16 ANSWER 74 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1971:141565 CAPLUS Full-text

DN 74:141565

TI Hypotensive 5,6,7a,8,11,11a,12,12a-octahydroindolo[2,1-a]isoquinolin-

9(10H)-ones

IN Shavel, John, Jr.; Morrison, Glenn Curtis

PA Warner-Lambert Pharmaceutical Co.

SO U.S., 5 pp. CODEN: USXXAM

DT Patent LA English

FAN.CNT 1

	<u>-</u>					
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	US 3557122	A	19710119	US 1968-766636	19681010	
PRAI	US 1968-766636		19681010			

IT 31804-77-0P

RN 31804-77-0 CAPLUS

CN 6-Isoquinolinol, 2-acetyl-1,2,3,4-tetrahydro-7-methoxy-1-[(4-oxo-2-cyclohexen-1-yl)methyl]-, acetate (ester) (8CI) (CA INDEX NAME)

L16 ANSWER 75 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1970:455982 CAPLUS Full-text

DN 73:55982

TI β -Stimulating 6,7-diacyloxy-1-(3,4,5-trimethoxybenzyl)-1,2,3,4-tetrahydroisoquinolines

IN Watanabe, Toshio; Tsukamoto, Goro; Hayashi, Kimiaki; Sato, Masanori; Toda,

Iwasawa

PA Tanabe Seiyaku Co., Ltd.

SO Ger. Offen., 20 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

PAIN.	CMT	T					
	PA!	TENT NO.	KIND	DATE	AP:	PLICATION NO.	DATE
ΡI	DE	1961947	A	19700618	DE	1969-1961947	19691210
	DE	1961947	B2	19740328			
	DE	1961947	C3	19741031			
	ΙL	33480	A1	19730330	ΙL	1969-33480	19691203
	US	3647799	A	19720307	US	1969-882296	19691204
	FΙ	49166	В	19741231	FI	1969-3512	19691204
	ES	374291	A1	19711216	ES	1969-374291	19691205
	BE	742807	A	19700514	BE	1969-742807	19691208
	GB	1242160	A	19710811	GB	1969-1242160	19691208
	NL	6918454	Α	19700612	NL	1969-18454	19691209

		2025778	,A5	19700910	FR	1969-42467	19691209
	FR 2	2025778	B1	19731221			
	AT 2	294095	В	19711110	ΑT	1969-11438	19691209
		347744	В	19720814	SE	1969-17003	19691209
	NO 1	126320	В	19730122	NO	1969-4860	19691209
	BR 6	5914920	A0	19730308	BR	1969-214920	19691209
	DK 1	L29994	В	19741209	DK	1969-6498	19691209
	CH 5	523250	A	19720531	CH	1969-523250	19691210
	CS 1	L56504	P	19740724	CS	1969-8138	19691210
PRAI	JP 1	L968-90741		19681210			
IT	2894	10-86-5P 28940	-88-71	28940-89-8P			
		10-90-1P 28940					
		4-29-2P 29051					
		21-51-7P 34221					
		SPN (Synthetic		aration); PREP	(Pr	eparation)	
RN	2894	0-86-5 CAPLUS	3				
CN	6,7-	Isoquinolinedi	iol. 1	,2,3,4-tetrahy	iro-	1- (3.4.5-trime	thovuhenzull-
	diac	etate (ester).	oxal	ate (1:1), (-)-	- (8	CT) (CA TNDEY	MAME!
		, , ,		(// (/	, ,	OI) (ON INDEX	. NAUL)
	CM	1					
	CRN	47685-00-7					
	CMF	C23 H27 N O7					

Rotation (-).

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 28940-88-7 CAPLUS
CN Butyric acid, 1,2,3,4-tetrahydro-1-(3,4,5-trimethoxybenzyl)-6,7isoquinolinediyl ester oxalate (1:1), (S)-(-)- (8CI) (CA INDEX NAME)

CM 1

CRN 39772-42-4
CMF C27 H35 N O7

Absolute stereochemistry.

CM 2

CRN 144-62-7 CMF C2 H2 O4

но-С-С-он

RN 28940-89-8 CAPLUS

CN Butyric acid, 1,2,3,4-tetrahydro-1-(3,4,5-trimethoxybenzyl)-6,7-isoquinolinediyl ester tartrate (1:1), (S)-(-)- (8CI) (CA INDEX NAME)

CM 1

CRN 39772-42-4 CMF C27 H35 N O7

Absolute stereochemistry.

CM 2

CRN 87-69-4 CMF C4 H6 O6

Absolute stereochemistry.

RN 28940-90-1 CAPLUS

CN Butyric acid, 1,2,3,4-tetrahydro-1-(3,4,5-trimethoxybenzyl)-6,7isoquinolinediyl ester succinate (1:1), (S)-(-)- (8CI) (CA INDEX NAME)

CM 1

CRN 39772-42-4 CMF C27 H35 N O7

Absolute stereochemistry.

CM 2

CRN 110-15-6 CMF C4 H6 O4

 $HO_2C-CH_2-CH_2-CO_2H$

RN 28940-91-2 CAPLUS

Isobutyric acid, 1,2,3,4-tetrahydro-1-(3,4,5-trimethoxybenzyl)-6,7-isoquinolinediyl ester oxalate (1:1), (-)- (8CI) (CA INDEX NAME)

CM 1

CRN 47765-21-9 CMF C27 H35 N O7

Rotation (-).

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 28954-28-1 CAPLUS

CN 2(1H)-Isoquinolinecarboxylic acid, 3,4-dihydro-6,7-dihydroxy-1-(3,4,5trimethoxybenzyl)-, benzyl ester, diacetate (ester), (-)- (8CI) (CA INDEX

NAME)

Rotation (-).

RN 28954-29-2 CAPLUS

CN 6,7-Isoquinolinediol, 1,2,3,4-tetrahydro-1-(3,4,5-trimethoxybenzyl)-, dipropionate (ester), oxalate (1:1), (-)- (8CI) (CA INDEX NAME)

CM 1

CRN 47730-19-8 CMF C25 H31 N O7

Rotation (-).

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 29051-20-5 CAPLUS

CN Butyric acid, 1,2,3,4-tetrahydro-1-(3,4,5-trimethoxybenzyl)-6,7-isoquinolinediyl ester maleate (1:1), (S)-(-)- (8CI) (CA INDEX NAME)

CM 1

CRN 39772-42-4 CMF C27 H35 N O7

Absolute stereochemistry.

CM 2

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.

RN 34202-91-0 CAPLUS
CN Butanoic acid, 1,2,3,4-tetrahydro-1-[(3,4,5-trimethoxyphenyl)methyl]-6,7isoquinolinediyl ester, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 47765-22-0
CMF C27 H35 N O7

CM 2

CRN 144-62-7 CMF C2 H2 O4

C23 H27 N O7

но-С-С-он

CMF

CM 2

CRN 144-62-7 CMF C2 H2 O4

но-С-С-он

RN 34221-52-8 CAPLUS

CN Propanoic acid, 2-methyl-, 1,2,3,4-tetrahydro-1-[(3,4,5-trimethoxyphenyl)methyl]-6,7-isoquinolinediyl ester, ethanedioate (1:1)

(9CI) (CA INDEX NAME)

CM 1

CRN 34685-11-5 CMF C27 H35 N O7

CM 2

CRN 144-62-7 CMF C2 H2 O4

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L16 ANSWER 76 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN
     1970:121744 CAPLUS Full-text
AN
DN
     72:121744
ΤI
     Synthetic studies of curare alkaloids. XIV. Synthesis of
     1-(4'-benzyloxybenzyl)6-methoxy-7-(2''-methoxy-5''-
     methoxycarbonylmethylphenoxy) -N-methyl-1,2,3,4-tetrahydroisoquinoline
     Tolkachev, O. N.; Volkova, L. V.; Vasil'ev, G. S.; Prokhorov, A. B.;
ΑU
     Kulachkina, N. S.; Preobrazhenskii, N. A.
CS
     Mosk. Inst. Tonkoi Khim. Tekhnol. im. Lomonosova, Moscow, USSR
     Khimiya Geterotsiklicheskikh Soedinenii (1969), (5), 831-7
SO
     CODEN: KGSSAQ; ISSN: 0132-6244
DT
     Journal
LΑ
     Russian
IT
     26626-00-6P 26626-03-9P 26648-66-8P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
RN
     26626-00-6 CAPLUS
    7-Isoquinolinol, 1-[p-(benzyloxy)benzyl]-1,2,3,4-tetrahydro-6-methoxy-
CN
     acetate (ester), oxalate (1:1), (\pm)- (8CI) (CA INDEX NAME)
     CM
         1
    CRN 96808-23-0
    CMF C26 H27 N O4
    Ph-CH2-
    CM
         2
    CRN 144-62-7
```

CMF C2 H2 O4

RN 26626-03-9 CAPLUS
CN 7-Isoquinolinol, 1-[p-(benzyloxy)benzyl]-1,2,3,4-tetrahydro-6-methoxy2methyl-, acetate (ester), hydrochloride, (±)- (8CI) (CA INDEX NAME)

HC1

RN 26648-66-8 CAPLUS

CN 7-Isoquinolinol, 1-[p-(benzyloxy)benzyl]-1,2,3,4-tetrahydro-6-methoxy-

methyl-, acetate (ester), oxalate (1:1), (\pm)- (8CI) (CA INDEX NAME)

CM 1

2-

CRN 4119-55-5 CMF C27 H29 N O4

CM 2

CRN 144-62-7 CMF C2 H2 O4

но-С-С-он

L16 ANSWER 77 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1970:43387 CAPLUS Full-text

DN 72:43387

TI Enzymic phenol oxidation. III. Head-to-head coupling of 1,2,3,4-tetrahydro-7-hydroxy-1-(4-hydroxyphenethyl)-6-methoxy-2-methylisoquinoline with homogenized Wasabia japonica and hydrogen peroxide

AU Kametani, Tetsuji; Takano, Seiichi; Kobari, Takashi

CS Pharm. Inst., Tohoku Univ., Sendai, Japan

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Journal of the Chemical Society [Section] C: Organic (1969), (19),
so
2770-3
     CODEN: JSOOAX; ISSN: 0022-4952
DT
     Journal
     English
T.A
IT
     25888-72-6P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
     25888-72-6 CAPLUS
RN
     7-Isoquinolinol, 1,2,3,4-tetrahydro-1-(p-hydroxyphenethyl)-6-methoxy-
CN
2-
     methyl-, diacetate (ester) (8CI) (CA INDEX NAME)
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L16 ANSWER 78 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN
AN
     1969:413241 CAPLUS Full-text
DN
     71:13241
    Alkaloid biosynthesis. XIV. Secologanin: its conversion into
ΤI
ipecoside
     and its role as biological precursor of the indole alkaloids
     Battersby, Alan R.; Burnett, Alan R.; Parsons, P. G.
     Univ. Liverpool, Liverpool, UK
SO
     Journal of the Chemical Society [Section] C: Organic (1969), (8),
1187-92
     CODEN: JSOOAX; ISSN: 0022-4952
DΤ
     Journal
LA
    English
IT
     21104-39-2P 21104-40-5P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
RN
     21104-39-2 CAPLUS
     2H-Pyran-5-carboxylic acid, 4-[[2-acetyl-6,7-bis(acetyloxy)-1,2,3,4-
CN
     tetrahydro-1-isoquinoliny1]methyl]-3-ethenyl-3,4-dihydro-2-[(2,3,4,6-
tetra-
     O-acetyl-\beta-D-glucopyranosyl)oxy]-, methyl ester, [2S-
     [2\alpha, 3\beta, 4\beta(S^*)] (9CI) (CA INDEX NAME)
```

RN 21104-40-5 CAPLUS

CN 2H-Pyran-5-carboxylic acid, 4-[[2-acetyl-6,7-bis(acetyloxy)-1,2,3,4-tetrahydro-1-isoquinolinyl]methyl]-3-ethenyl-3,4-dihydro-2-[(2,3,4,6-tetra-

O-acetyl- β -D-glucopyranosyl)oxy]-, methyl ester, [2S-[2 α , 3 β , 4 β (R*)]]- (9CI) (CA INDEX NAME)

AcO CH2 OAC

$$AcO$$
 CH2 C CH2 C AcO

 AcO AcO

 AcO AcO

L16 ANSWER 79 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1969:403289 CAPLUS Full-text

DN 71:3289

TI 1-Benzyl-6,7-di(lower-alkanoyloxy)-1,2,3,4-tetrahydroisoquinolines

IN Yamato, Eisaku; Kasuya, Shoichi

PA Tanabe Seiyaku Co., Ltd.

SO Jpn. Tokkyo Koho, 2 pp. CODEN: JAXXAD

DE Detent

DT Patent

LA Japanese

FAN.CNT 1

IT 22655-30-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 22655-30-7 CAPLUS

CN 6,7-Isoquinolinediol, 1-benzyl-1,2,3,4-tetrahydro-, diacetate (ester), sulfate (1:1) (8CI) (CA INDEX NAME)

CM 1

CRN 47446-88-8 CMF C20 H21 N O4

CM 2

CRN 7664-93-9 CMF H2 O4 S

L16 ANSWER 80 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN AN1969:20259 CAPLUS Full-text DN 70:20259 ΤI Preparation of secologanin: its conversion into ipecoside and its role in indole alkaloid biosynthesis Battersby, Alan R.; Burnett, Alan R.; Parsons, P. G. ΑU Univ. Liverpool, Liverpool, UK CS so Chemical Communications (London) (1968), (21), 1280-1 CODEN: CCOMA8; ISSN: 0009-241X DΤ Journal LA English 21104-39-2P 21104-40-5P IT RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) RN21104-39-2 CAPLUS 2H-Pyran-5-carboxylic acid, 4-[[2-acetyl-6,7-bis(acetyloxy)-1,2,3,4-CNtetrahydro-1-isoquinolinyl]methyl]-3-ethenyl-3,4-dihydro-2-[(2,3,4,6tetra-O-acetyl- β -D-glucopyranosyl)oxy]-, methyl ester, [2S- $[2\alpha, 3\beta, 4\beta(s^*)]$ (9CI) (CA INDEX NAME)

RN 21104-40-5 CAPLUS

CN 2H-Pyran-5-carboxylic acid, 4-[[2-acetyl-6,7-bis(acetyloxy)-1,2,3,4-tetrahydro-1-isoquinolinyl]methyl]-3-ethenyl-3,4-dihydro-2-[(2,3,4,6-tetra-

O-acetyl- β -D-glucopyranosyl)oxy]-, methyl ester, [2S-[2 α , 3 β , 4 β (R*)]]- (9CI) (CA INDEX NAME)

AcO CH2 OAC

$$AcO$$
 CH2 C CH2 C AcO

 AcO AcO

 AcO AcO AcO AcO AcO

L16 ANSWER 81 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1968:459456 CAPLUS Full-text

DN 69:59456

TI Alkaloids of Xylopia papuana

AU Johns, S. R.; Lamberton, J. A.; Sioumis, A. A.

CS Div. Appl. Chem., C.S.I.R.O., Melbourne, Australia

SO Australian Journal of Chemistry (1968), 21(5), 1383-6 CODEN: AJCHAS; ISSN: 0004-9425

DT Journal

LA English

IT 14199-49-6P 19894-20-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 14199-49-6 CAPLUS

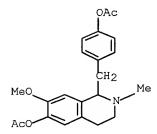
CN Reticuline, diacetate (ester) (8CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 19894-20-3 CAPLUS
CN 7-Isoquinolinol, 2-acetyl-1-[[(4-acetyloxy)phenyl]methyl]-1,2-dihydro6methoxy-, acetate (ester), (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L16 ANSWER 82 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN AN 1968:427560 CAPLUS Full-text DN 69:27560 TI Studies on the syntheses of heterocyclic compounds. CCIX. Total syntheses of (+-)-isococlaurine and (-)-lotusine ΑU Kametani, Tetsuji; Takano, Seiichi; Sasaki, Fujinori; Yamaki, Kazuya CS Tohoku Univ. Sch. Med., Sendai, Japan SO Chemical & Pharmaceutical Bulletin (1968), 16(1), 20-4CODEN: CPBTAL; ISSN: 0009-2363 DTJournal LA English ΙT 19442-72-9P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) RN 19442-72-9 CAPLUS CN Butanedioic acid, 2,3-bis(benzoyloxy)-, [S-(R*,R*)]-, compd. with 1-[[4-(acetyloxy)phenyl]methyl]-1,2,3,4-tetrahydro-7-methoxy-2-methylisoquinolinyl acetate (ester) (9CI) (CA INDEX NAME) CM 1 CRN 47581-12-4 CMF C22 H25 N O5



CM 2

CRN 17026-42-5 CMF C18 H14 O8

Absolute stereochemistry. Rotation (+).

L16 ANSWER 83 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1968:104952 CAPLUS Full-text

DN 68:104952

TI Synthesis of 6,7-dihydroxy-1,2,3,4-tetrahydroisoquinoline derivatives

AU Yamato, Eisaku; Mashimo, Kiyohiko; Hirakura, Minoru; Yamagata, Osamu; Kurihara, Sumio

CS Tanabe Seiyaku Co., Ltd., Osaka, Japan

SO Yakugaku Zasshi (1967), 87(9), 1083-8 CODEN: YKKZAJ; ISSN: 0031-6903

DT Journal

LA Japanese

IT 18063-81-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 18063-81-5 CAPLUS

CN Isoquinoline, 2-acetyl-1,2,3,4-tetrahydro-6,7-dihydroxy-1-(3,4,5-trimethoxybenzyl)-, diacetate (ester) (8CI) (CA INDEX NAME)

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L16 ANSWER 84 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN
AN
    1968:29924 CAPLUS Full-text
    68:29924
DN
ΤI
    1-Phenethylisoquinoline alkaloids. I. Structure and synthesis of
     (-)-melanthioidine, a bisphenethylisoquinoline alkaloid
ΑU
    Battersby, Alan R.; Herbert, Richard B.; Mo, Lucy; Santavy, Frantisek
CS
    Univ. Liverpool, Liverpool, UK
    Journal of the Chemical Society [Section] C: Organic (1967), (18),
SO
    1739-44
    CODEN: JSOOAX; ISSN: 0022-4952
DT
    Journal
LA
    English
OS
    CASREACT 68:29924
IT
    17801-29-5P
    RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
RN
    17801-29-5 CAPLUS
    7-Isoquinolinol, 1-[4-(benzyloxy)-3-bromophenethyl]-1,2,3,4-
tetrahydro-6-
    methoxy-2-methyl-, acetate (ester), hydrochloride, (±)- (8CI)
```

INDEX NAME)

● HCl

L16 ANSWER 85 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1967:490969 CAPLUS <u>Full-text</u>
DN 67:90969

TI 1-Benzyl-1,2,3,4-tetrahydroisoquinoline alkaloids from Alseodaphne archboldiana

AU Johns, Stanley R.; Lamberton, John A.; Sioumis, A. A.

CS Div. Appl. Chem., C.S.I.R.O., Melbourne, Australia

SO Australian Journal of Chemistry (1967), 20(8), 1729-35

CODEN: AJCHAS; ISSN: 0004-9425

DT Journal

LA English

IT 3422-43-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 3422-43-3 CAPLUS

CN 7-Isoquinolinol, 2-acetyl-1-[[4-(acetyloxy)phenyl]methyl]-1,2,3,4-tetrahydro-6-methoxy-, acetate (ester), (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L16 ANSWER 86 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1967:454293 CAPLUS Full-text

DN 67:54293

TI Cassytha alkaloids. IV. Alkaloids of Cassytha racemosa

AU Johns, Stanley R.; Lamberton, John A.; Sioumis, A. A.

CS Div. Appl. Chem., C.S.I.R.O., Melbourne, Australia

SO Australian Journal of Chemistry (1967), 20(7), 1457-62 CODEN: AJCHAS; ISSN: 0004-9425

DT Journal

LA English

IT 3422-43-3P

RL: PREP (Preparation)

(from Cassytha racemosa)

RN 3422-43-3 CAPLUS

CN 7-Isoquinolinol, 2-acetyl-1-[[4-(acetyloxy)phenyl]methyl]-1,2,3,4-tetrahydro-6-methoxy-, acetate (ester), (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L16 ANSWER 87 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1967:2672 CAPLUS Full-text

66:2672 DN ΤI Phenol oxidation. I. The synthesis of isoboldine and glaucine Jackson, Anthony Hugh; Martin, Joseph Armstrong ΑU Univ. Liverpool, Liverpool, UK CS Journal of the Chemical Society [Section] C: Organic (1966), (22), so 2061-9 CODEN: JSOOAX; ISSN: 0022-4952 DTJournal English LACASREACT 66:2672 OS IT 13261-09-1P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) RN 13261-09-1 CAPLUS 7-Isoquinolinol, 1,2,3,4-tetrahydro-6-methoxy-2-methyl-1-vanillyl-, CN diacetate (ester), monopicrate (8CI) (CA INDEX NAME) CM 1 47653-34-9 CRN CMF C23 H27 N O6

CM 2

CRN 88-89-1 CMF C6 H3 N3 O7

L16 ANSWER 88 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN AN1965:480864 CAPLUS Full-text 63:80864 DNOREF 63:14929e-h Constitution of thalsimine TI ΑU Maekh, S. Kh.; Yunusov, S. Yu. Inst. Chem. Vegetable Compounds, Tashkent CS Khim. Prirodn. Soedin., Akad. Nauk Uz. SSR (1965), (3), 188-94 so \mathbf{DT} Journal

L16 ANSWER 89 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN AN1965:51864 CAPLUS Full-text DN 62:51864 OREF 62:9184b-d Alkaloids of Nelumbo nucifera. IV. Total synthesis of liensinine Hsieh, Yu-Yuan; Pan, Pei-Chuan; Chen, Wen-Chi; Kao, Yee-Sheng SO Scientia Sinica (English Edition) (1964), 12(12), 2020-5 CODEN: SSINAV; ISSN: 0582-236X DT Journal LA English 1857-42-7, 7-Isoquinolinol, 1-[p-(benzyloxy)benzyl]-1,2,3,4tetrahydro-6-methoxy-, acetate (ester), (+)- 1857-43-8, 7-Isoquinolinol, 1-[p-(benzyloxy)benzyl]-1,2,3,4-tetrahydro-6-methoxyacetate (ester), (-)- 4119-55-5, 7-Isoquinolinol, 1-[p-(benzyloxy)benzyl]-1,2,3,4-tetrahydro-6-methoxy-2-methyl-, acetate (ester) (preparation of) 1857-42-7 CAPLUS CN 7-Isoquinolinol, 1-[p-(benzyloxy)benzyl]-1,2,3,4-tetrahydro-6-methoxyacetate (ester), (+)- (8CI) (CA INDEX NAME) Rotation (+).

RN 1857-43-8 CAPLUS
CN 7-Isoquinolinol, 1-[p-(benzyloxy)benzyl]-1,2,3,4-tetrahydro-6-methoxy,
acetate (ester), (-)- (8CI) (CA INDEX NAME)

Rotation (-).

RN 4119-55-5 CAPLUS
CN 7-Isoquinolinol, 1-[p-(benzyloxy)benzyl]-1,2,3,4-tetrahydro-6-methoxy2methyl-, acetate (ester) (8CI) (CA INDEX NAME)

L16 ANSWER 90 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN AN 1965:36788 CAPLUS Full-text 62:36788 DN OREF 62:6471a-f Reaction of flavanone with hydrazine ΤI ΑU Kallay, F.; Janzo, G.; Koczor, I. Res. Inst. Org. Chem. Ind., Budapest, Hung. so Tetrahedron (1965), 21(1), 19-24 CODEN: TETRAB; ISSN: 0040-4020 DT Journal LA Unavailable os CASREACT 62:36788 IT 1692-42-8, Acetamide, N-(α -phenethylsalicyl)-, acetate (preparation of) RN 1692-42-8 CAPLUS Acetamide, N- $(\alpha$ -phenethylsalicyl)-, acetate (7CI, 8CI) (CA INDEX CN NAME)

L16 ANSWER 91 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1964:45659 CAPLUS Full-text

DN 60:45659

OREF 60:8004a-e

FI 6(or 7)-Hydroxy-1,2,3,4-tetrahydroisoquinolines

PA F. Hoffmann-La Roche & Co., A.-G.

SO 19 pp.

DT Patent

LA Unavailable

LA	PATENT NO.	KIND	DATE	APPLICATION 1	NO. DATE
PI	BE 627177		196307	16 BE	
	FR 1344709			FR	
	FR M2303			FR	
	GB 995369			GB	
	GB 995370			GB	
	US 3217007		1965	US	
PRAI			196201		
IT	94760-32-4 , 7	-Isoquinol	linol,	1-(p-chlorophenethyl)	-1,2,3,4-

IT 94760-32-4, 7-Isoquinolinol, 1-(p-chlorophenethyl)-1,2,3,4tetrahydro-6-methoxy-2-methyl-, acetate

(preparation of) RN 94760-32-4 CAPLUS

CN 7-Isoquinolinol, 1-(p-chlorophenethyl)-1,2,3,4-tetrahydro-6-methoxy-2methyl-, acetate (7CI) (CA INDEX NAME)

L16 ANSWER 92 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1963:403691 CAPLUS Full-text

DN 59:3691

OREF 59:691g-h,692a-d

TI (-)-N-Methylcoclaurine from Phylica rogersii

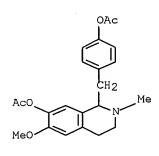
AU Arndt, R. R.

CS S. African Council Sci. Ind. Res., Pretoria

SO Journal of the Chemical Society, Abstracts (1963) 2547-9 CODEN: JCSAAZ; ISSN: 0590-9791

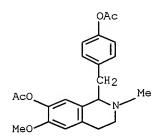
DT Journal

LA Unavailable



● HCl

RN 95133-87-2 CAPLUS
CN 7-Isoquinolinol, 1,2,3,4-tetrahydro-1-(p-hydroxybenzyl)-6-methoxy-2-methyl, diacetate (7CI) (CA INDEX NAME)



L16 ANSWER 93 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN AN1961:67220 CAPLUS Full-text 55:67220 DN OREF 55:12781b-d Recovery of a glucoside from ipecac Bellet, Paul PA UCLAF DΤ Patent LΑ Unavailable FAN.CNT 1 APPLICATION NO. DATE PATENT NO. KIND DATE ΡI DE

PI DE 1060089 19590625 II **21104-39-2**, Ipecoside, hexaacetate

(isolation from ipecac)

RN 21104-39-2 CAPLUS

CN 2H-Pyran-5-carboxylic acid, 4-[[2-acetyl-6,7-bis(acetyloxy)-1,2,3,4-tetrahydro-1-isoquinolinyl]methyl]-3-ethenyl-3,4-dihydro-2-[(2,3,4,6-tetra-

O-acetyl- β -D-glucopyranosyl)oxy]-, methyl ester, [2S-[2 α , 3 β , 4 β (S*)]]- (9CI) (CA INDEX NAME)

L16 ANSWER 94 OF 94 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1955:21606 CAPLUS Full-text

DN 49:21606

OREF 49:4233i,4234a-b

TI Ipecoside

AU Bellet, Paul

CS Roussel-Uclaf, Paris-Romainville

SO Annales Pharmaceutiques Françaises (1954), 12, 466-70 CODEN: APFRAD; ISSN: 0003-4509

DT Journal

LA Unavailable

IT 21104-39-2, Ipecoside, hexaacetate

(preparation of)

RN 21104-39-2 CAPLUS

CN 2H-Pyran-5-carboxylic acid, 4-[[2-acetyl-6,7-bis(acetyloxy)-1,2,3,4-tetrahydro-1-isoquinolinyl]methyl]-3-ethenyl-3,4-dihydro-2-[(2,3,4,6-tetra-

O-acetyl- β -D-glucopyranosyl)oxy]-, methyl ester, [2S-[2 α , 3 β , 4 β (S*)]]- (9CI) (CA INDEX NAME)

=> logoff hold

SEARCH 2 CAS REGISTRY

=> fil req Uploading E:\express6\Queries\rogers2005\metX10X2S.str MY "3 15 45 ак—жи ^{* 7} -54 A 7 AK * 3 AK 1 H 4 2 17 AH2 12 11 c, a o-*" 4-1B chain nodes : 7 8 12 13 14 15 16 17 18 19 26 27 28 29 30 34 35 36 37 38 39 45 47 48 49 52 54 55 ring nodes : 1 2 3 4 5 6 ring/chain nodes : 25 53 chain bonds : 2-13 13-15 14-15 15-16 25-26 26-45 28-29 28-30 34-35 36-37 38-39 38-52 47-48 48-49 54-55 ring/chain bonds : 6-25 25-53 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 exact/norm bonds : 2-13 6-25 13-15 14-15 15-16 25-26 25-53 26-45 28-29 28-30 34-35 36-37 38-39 38-52 47-48 48-49 54-55 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6 G1:[*1],[*2] G4: [*3], [*4], [*5], [*6], [*7] G9: [*8], [*9], [*10], [*11] G10:H, [*12] Connectivity: 7:1 E exact RC ring/chain 17:1 E exact RC ring/chain 26:2 E exact RC ring/chain 29:1 E exact RC ring/chain 30:1 E exact RC ring/chain 49:1 E exact RC ring/chain 55:1 E exact RC ring/chain Match level : 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:Atom 24:CLASS 25:CLASS 26:CLASS 27:Atom 28:CLASS 29:CLASS 30:CLASS 34:CLASS 35:Atom 36:CLASS 37:Atom 38:CLASS 39:Atom 45:CLASS 47:CLASS 48:CLASS 49:CLASS 52:CLASS 53:CLASS 54:CLASS 55:CLASS Generic attributes : Number of Carbon Atoms: less than 7 Number of Carbon Atoms: less than 7 19: Saturation : Saturated

26:

```
Number of Carbon Atoms : less than 7
```

27:

Saturation : Unsaturated

29:

Number of Carbon Atoms : less than 7

30:

Number of Carbon Atoms : less than 7

35:

Saturation : Unsaturated

37:

Saturation : Unsaturated

39:

Saturation : Unsaturated

49:

Number of Carbon Atoms : less than 7

55:

Number of Carbon Atoms : less than 7

Element Count :
Node 19: Limited

N,N1

L1 STRUCTURE UPLOADED

=> d

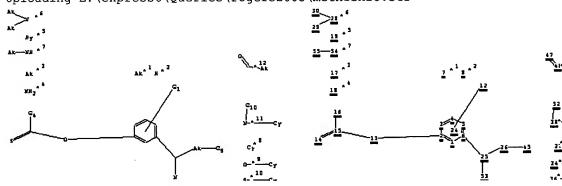
L1 HAS NO ANSWERS

L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

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chain nodes :

7 8 12 13 14 15 16 17 18 19 26 27 28 29 30 34 35 36 37 38 39

45 47 48 49 52 54 55

ring nodes:

1 2 3 4 5 6

ring/chain nodes :

25 53

chain bonds :

2-13 13-15 14-15 15-16 25-26 26-45 28-29 28-30 34-35 36-37 38-39 38-52

47-48 48-49 54-55

ring/chain bonds :

```
6-25 25-53
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
2-13 6-25 13-15 14-15 15-16 25-26 25-53 26-45 28-29 28-30 34-35 36-37
38-39 38-52 47-48 48-49 54-55
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
G1:[*1],[*2]
G4: [*3], [*4], [*5], [*6], [*7]
G9: [*8], [*9], [*10], [*11]
G10:H, [*12]
Connectivity:
7:1 E exact RC ring/chain 17:1 E exact RC ring/chain 26:2 E exact RC ring/chain
29:1 E exact RC ring/chain 30:1 E exact RC ring/chain 49:1 E exact RC
ring/chain 55:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 12:CLASS
13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:Atom 24:CLASS
25:CLASS 26:CLASS 27:Atom 28:CLASS 29:CLASS 30:CLASS 34:CLASS 35:Atom
36:CLASS 37:Atom 38:CLASS 39:Atom 45:CLASS 47:CLASS 48:CLASS 49:CLASS
52:CLASS 53:CLASS 54:CLASS 55:CLASS
Generic attributes :
7:
Number of Carbon Atoms : less than 7
17:
Number of Carbon Atoms : less than 7
19:
Saturation
                     : Saturated
26:
Number of Carbon Atoms : less than 7
Saturation
                     : Unsaturated
Number of Carbon Atoms: less than 7
Number of Carbon Atoms : less than 7
35:
Saturation
                     : Unsaturated
37:
Saturation
                     : Unsaturated
39:
Saturation
                     : Unsaturated
49:
Number of Carbon Atoms: less than 7
Number of Carbon Atoms : less than 7
Element Count :
Node 19: Limited
   N,N1
```

```
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                                         19 * 3
                Ak* H * 2
                              c, ª
chain nodes :
7 8 12 13 14 15 16 17 18 19 26 27 28 29
                                                  30
                                                       34
                                                          35
                                                              36 37 38
45 47 48 49 52 54 55
ring nodes :
1 2 3 4 5 6
ring/chain nodes :
25 53
chain bonds :
2-13 13-15 14-15 15-16 25-26 26-45 28-29 28-30 34-35 36-37 38-39 38-52
47-48 48-49 54-55
ring/chain bonds :
6-25 25-53
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
2-13 6-25 13-15 14-15 15-16 25-26 25-53 26-45 28-29 28-30 34-35 36-37
38-39 38-52 47-48 48-49 54-55
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
G1:[*1],[*2]
G4:[*3],[*4],[*5],[*6],[*7]
G9: [*8], [*9], [*10], [*11]
G10:H, [*12]
Connectivity:
7:1 E exact RC ring/chain 17:1 E exact RC ring/chain 26:2 E exact RC ring/chain
29:1 E exact RC ring/chain 30:1 E exact RC ring/chain 49:1 E exact RC
ring/chain 55:1 E exact RC ring/chain
Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 12:CLASS
13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:Atom 24:CLASS
25:CLASS 26:CLASS 27:Atom 28:CLASS 29:CLASS 30:CLASS 34:CLASS 35:Atom
36:CLASS 37:Atom 38:CLASS 39:Atom 45:CLASS 47:CLASS 48:CLASS 49:CLASS
52:CLASS 53:CLASS 54:CLASS 55:CLASS
Generic attributes :
7:
Number of Carbon Atoms: less than 7
17:
Number of Carbon Atoms: less than 7
19:
                      : Saturated
Saturation
26:
Number of Carbon Atoms : less than 7
```

27:

Saturation : Unsaturated

29:

Number of Carbon Atoms : less than 7

30:

Number of Carbon Atoms : less than 7

35:

Saturation : Unsaturated

37:

Saturation : Unsaturated

39:

Saturation : Unsaturated

49:

Number of Carbon Atoms : less than 7

55:

Number of Carbon Atoms : less than 7

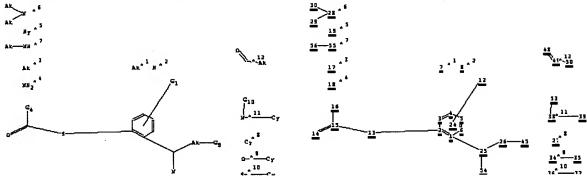
Element Count : Node 19: Limited

N,N1

L3 STRUCTURE UPLOADED

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chain nodes :

7 8 12 13 14 15 16 17 18 19 26 27 28 29 30 34 35 36 37 38 39

45 48 49 50 53 55 56

ring nodes :

1 2 3 4 5 6

ring/chain nodes :

25 54

chain bonds :

2-13 13-15 14-15 15-16 25-26 26-45 28-29 28-30 34-35 36-37 38-39 38-53

48-49 49-50 55-56

ring/chain bonds :

1-25 25-54

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

1-25 2-13 13-15 14-15 15-16 25-26 25-54 26-45 28-29 28-30 34-35 36-37

38-39 38-53 48-49 49-50 55-56

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

```
G1:[*1],[*2]
G4:[*3],[*4],[*5],[*6],[*7]
G9: [*8], [*9], [*10], [*11]
G10:H,[*12]
Connectivity:
7:1 E exact RC ring/chain 17:1 E exact RC ring/chain 26:2 E exact RC ring/chain
29:1 E exact RC ring/chain 30:1 E exact RC ring/chain 50:1 E exact RC ring/chain 56:1 E exact RC ring/chain
Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 12:CLASS
13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:Atom 24:CLASS 25:CLASS 26:CLASS 27:Atom 28:CLASS 29:CLASS 30:CLASS 34:CLASS 35:Atom 36:CLASS 37:Atom 38:CLASS 39:Atom 45:CLASS 48:CLASS 49:CLASS 50:CLASS 53:CLASS 54:CLASS 55:CLASS 56:CLASS
Generic attributes :
7:
Number of Carbon Atoms : less than 7
Number of Carbon Atoms : less than 7
19:
Saturation
                     : Saturated
26:
Number of Carbon Atoms : less than 7
Saturation
                         : Unsaturated
29:
Number of Carbon Atoms : less than 7
Number of Carbon Atoms : less than 7
35:
Saturation
                          : Unsaturated
37:
                : Unsaturated
Saturation
39:
Saturation
                          : Unsaturated
Number of Carbon Atoms : less than 7
Number of Carbon Atoms : less than 7
Element Count :
Node 19: Limited
    N,N1
```

L4 STRUCTURE UPLOADED

=>

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```
1,11
                              c, i
                              0-^<del>1</del>
                              e-* 10
chain nodes :
7 8 12 13 14 15 16 17 18 19 26 27 28 29 30 34 35 36 37 38 39
45 48 49 50 53 55 56
ring nodes :
1 2 3 4 5 6
ring/chain nodes :
chain bonds :
2-13 13-15 14-15 15-16 25-26 26-45 28-29 28-30 34-35 36-37 38-39 38-53
48-49 49-50 55-56
ring/chain bonds :
1-25 25-54
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-25 2-13 13-15 14-15 15-16 25-26 25-54 26-45 28-29 28-30 34-35 36-37
38-39 38-53 48-49 49-50 55-56
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
G1:[*1],[*2]
G4: [*3], [*4], [*5], [*6], [*7]
G9: [*8], [*9], [*10], [*11]
G10:H, [*12]
Connectivity:
7:1 E exact RC ring/chain 17:1 E exact RC ring/chain 26:2 E exact RC ring/chain
29:1 E exact RC ring/chain 30:1 E exact RC ring/chain 50:1 E exact RC
ring/chain 56:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 12:CLASS
13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:Atom 24:CLASS
25:CLASS 26:CLASS 27:Atom 28:CLASS 29:CLASS 30:CLASS 34:CLASS 35:Atom
36:CLASS 37:Atom 38:CLASS 39:Atom 45:CLASS 48:CLASS 49:CLASS 50:CLASS
53:CLASS 54:CLASS 55:CLASS 56:CLASS
Generic attributes :
7:
Number of Carbon Atoms: less than 7
17:
Number of Carbon Atoms : less than 7
19:
Saturation
                      : Saturated
26:
Number of Carbon Atoms : less than 7
27:
             : Unsaturated
Saturation
29:
```

```
Number of Carbon Atoms : less than 7
Number of Carbon Atoms : less than 7
35:
Saturation
                       : Unsaturated
37:
Saturation
                       : Unsaturated
39:
Saturation
                       : Unsaturated
50:
Number of Carbon Atoms : less than 7
56:
Number of Carbon Atoms : less than 7
Element Count :
Node 19: Limited
   N,N1
```

L5 STRUCTURE UPLOADED

G4:[*3],[*4],[*5],[*6],[*7]

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```
G9: [*8], [*9], [*10], [*11]
G10:H,[*12]
Connectivity:
7:1 E exact RC ring/chain 17:1 E exact RC ring/chain 26:2 E exact RC ring/chain
29:1 E exact RC ring/chain 30:1 E exact RC ring/chain 50:1 E exact RC
ring/chain 56:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:Atom 24:CLASS 25:CLASS 26:CLASS 27:Atom 28:CLASS 29:CLASS 30:CLASS 34:CLASS 35:Atom 36:CLASS 37:Atom 38:CLASS 39:Atom 45:CLASS 48:CLASS 49:CLASS 50:CLASS 53:CLASS 54:CLASS 55:CLASS 56:CLASS
Generic attributes :
Number of Carbon Atoms : less than 7
17:
Number of Carbon Atoms : less than 7
19:
Saturation
                     : Saturated
26:
Number of Carbon Atoms : less than 7
27:
Saturation
                     : Unsaturated
29:
Number of Carbon Atoms : less than 7
Number of Carbon Atoms : less than 7
35:
                           : Unsaturated
Saturation
37:
                  : Unsaturated
Saturation
39:
                           : Unsaturated
Saturation
Number of Carbon Atoms : less than 7
Number of Carbon Atoms : less than 7
Element Count :
Node 19: Limited
     N,N1
```

L6 STRUCTURE UPLOADED

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```
Ak<sup>1</sup> µ ^ 2
                                         18
                              4-^-<sup>10</sup>
chain nodes :
7 8 12 13 14 15 16 17 18 19 26 27 28 29 30 34 35 36 37 38 39
45 48 49 50 53 55 56
ring nodes :
1 2 3 4 5 6
ring/chain nodes :
25 54
chain bonds :
2-13 13-15 14-15 15-16 25-26 26-45 28-29 28-30 34-35 36-37 38-39 38-53
48-49 49-50 55-56
ring/chain bonds :
5-25 25-54
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
2-13 5-25 13-15 14-15 15-16 25-26 25-54 26-45 28-29 28-30 34-35 36-37
38-39 38-53 48-49 49-50 55-56
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
G1: [*1], [*2]
G4: [*3], [*4], [*5], [*6], [*7]
G9: [*8], [*9], [*10], [*11]
G10:H, [*12]
Connectivity:
7:1 E exact RC ring/chain 17:1 E exact RC ring/chain 26:2 E exact RC ring/chain
29:1 E exact RC ring/chain 30:1 E exact RC ring/chain 50:1 E exact RC
ring/chain 56:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 12:CLASS
13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:Atom 24:CLASS
25:CLASS 26:CLASS 27:Atom 28:CLASS 29:CLASS 30:CLASS 34:CLASS 35:Atom
36:CLASS 37:Atom 38:CLASS 39:Atom 45:CLASS 48:CLASS 49:CLASS 50:CLASS
53:CLASS 54:CLASS 55:CLASS 56:CLASS
Generic attributes :
7:
Number of Carbon Atoms : less than 7
17:
Number of Carbon Atoms : less than 7
19:
                      : Saturated
Saturation
26:
Number of Carbon Atoms : less than 7
27:
              : Unsaturated
Saturation
29:
```

```
Number of Carbon Atoms : less than 7
30:
Number of Carbon Atoms : less than 7
35:
                       : Unsaturated
Saturation
37:
Saturation
                       : Unsaturated
39:
Saturation
                       : Unsaturated
50:
Number of Carbon Atoms : less than 7
56:
Number of Carbon Atoms : less than 7
Element Count :
Node 19: Limited
   N,N1
```

L7 STRUCTURE UPLOADED

=> Uploading E:\express6\Queries\rogers2005\parX1SX2O.str 15 · 5 AK* 1 H * 2 5-^-¹⁰ chain nodes : 35 36 37 38 39 7 8 12 13 14 15 16 17 18 19 26 27 28 29 30 34 45 48 49 50 53 55 56 ring nodes : 1 2 3 4 5 6 ring/chain nodes : 25 54 chain bonds : 2-13 13-15 14-15 15-16 25-26 26-45 28-29 28-30 34-35 36-37 38-39 38-53 48-49 49-50 55-56 ring/chain bonds : 5-25 25-54 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 exact/norm bonds : 2-13 5-25 13-15 14-15 15-16 25-26 25-54 26-45 28-29 28-30 34-35 36-37 38-39 38-53 48-49 49-50 55-56 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6

G1:[*1],[*2]

G4:[*3],[*4],[*5],[*6],[*7]

```
G9: [*8], [*9], [*10], [*11]
G10:H,[*12]
Connectivity:
7:1 E exact RC ring/chain 17:1 E exact RC ring/chain 26:2 E exact RC ring/chain
29:1 E exact RC ring/chain 30:1 E exact RC ring/chain 50:1 E exact RC
ring/chain 56:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 12:CLASS
13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:Atom 24:CLASS
25:CLASS 26:CLASS 27:Atom 28:CLASS 29:CLASS 30:CLASS 34:CLASS 35:Atom
36:CLASS 37:Atom 38:CLASS 39:Atom 45:CLASS 48:CLASS 49:CLASS 50:CLASS 53:CLASS 54:CLASS 55:CLASS 56:CLASS
Generic attributes :
7:
Number of Carbon Atoms : less than 7
17:
Number of Carbon Atoms : less than 7
19:
Saturation
                : Saturated
26:
Number of Carbon Atoms : less than 7
27:
Saturation
                 : Unsaturated
29:
Number of Carbon Atoms : less than 7
Number of Carbon Atoms : less than 7
35:
Saturation
                     : Unsaturated
37:
                     : Unsaturated
Saturation
39:
                     : Unsaturated
Saturation
Number of Carbon Atoms : less than 7
Number of Carbon Atoms : less than 7
Element Count :
Node 19: Limited
   N,N1
```

L8 STRUCTURE UPLOADED

=>

Uploading E:\express6\Queries\rogers2005\parX1SX2S.str

```
2 *1 3 *2
                                         12 * 4
                              <u>, 11</u>
                              s-*-<sup>10</sup>
chain nodes :
7 8 12 13 14 15 16 17 18 19 26 27 28 29 30 34 35
                                                              36 37 38 39
45 48 49 50 53 55 56
ring nodes :
1 2 3 4 5
ring/chain nodes :
25 54
chain bonds :
2-13 13-15 14-15 15-16 25-26 26-45 28-29 28-30 34-35 36-37 38-39 38-53
48-49 49-50 55-56
ring/chain bonds :
5-25 25-54
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
2-13 5-25 13-15 14-15 15-16 25-26 25-54 26-45 28-29 28-30 34-35 36-37
38-39 38-53 48-49 49-50 55-56
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
G1:[*1],[*2]
G4: [*3], [*4], [*5], [*6], [*7]
G9: [*8], [*9], [*10], [*11]
G10:H, [*12]
Connectivity:
7:1 E exact RC ring/chain 17:1 E exact RC ring/chain 26:2 E exact RC ring/chain
29:1 E exact RC ring/chain 30:1 E exact RC ring/chain 50:1 E exact RC
ring/chain 56:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 12:CLASS
13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:Atom 24:CLASS
25:CLASS 26:CLASS 27:Atom 28:CLASS 29:CLASS 30:CLASS 34:CLASS 35:Atom
36:CLASS 37:Atom 38:CLASS 39:Atom 45:CLASS 48:CLASS 49:CLASS 50:CLASS
53:CLASS 54:CLASS 55:CLASS 56:CLASS
Generic attributes :
7:
Number of Carbon Atoms : less than 7
17:
Number of Carbon Atoms : less than 7
19:
                     : Saturated
Saturation
26:
Number of Carbon Atoms : less than 7
27:
             : Unsaturated
Saturation
29:
```

Number of Carbon Atoms : less than 7

30:

Number of Carbon Atoms : less than 7

35:

Saturation : Unsaturated

37:

Saturation : Unsaturated

39:

Saturation : Unsaturated

Number of Carbon Atoms : less than 7

Number of Carbon Atoms : less than 7

Element Count : Node 19: Limited

N,N1

L9 STRUCTURE UPLOADED

=> s (11 or 12 or 13 or 14 or 15 or 16 or 17 or 18 or 19) sss sam SAMPLE SEARCH INITIATED 18:13:21 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 3199 TO ITERATE

62.5% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE** BATCH **COMPLETE**

PROJECTED ITERATIONS: 60588 TO 67372 PROJECTED ANSWERS: 0 TO

O SEA SSS SAM (L1 OR L2 OR L3 OR L4 OR L5 OR L6 OR L7 OR L8 OR L9 L10

=> s (11 or 12 or 13 or 14 or 15 or 16 or 17 or 18 or 19) sss full FULL SEARCH INITIATED 18:13:36 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 62536 TO ITERATE

100.0% PROCESSED 62536 ITERATIONS 0 ANSWERS

0 ANSWERS

SEARCH TIME: 00.00.03

O SEA SSS FUL (L1 OR L2 OR L3 OR L4 OR L5 OR L6 OR L7 OR L8 OR L9 L11

=> log h

SEARCH 2 HARPAT

=> fil marpat. => Uploading E:\express6\Queries\rogers2005\metX10X2Smar.str 13 [11 chain nodes : 7 8 12 13 14 15 16 17 18 19 26 27 28 29 30 34 35 36 37 38 39 45 47 48 49 52 54 55 ring nodes : 1 2 3 4 5 ring/chain nodes : chain bonds : 2-13 6-25 13-15 14-15 15-16 25-26 25-53 26-45 28-29 28-30 34-35 36-37 38-39 38-52 47-48 48-49 54-55 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 exact/norm bonds : 2-13 6-25 13-15 14-15 15-16 25-26 25-53 26-45 28-29 28-30 34-35 36-37 38-39 38-52 47-48 48-49 54-55 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6 G1: [*1], [*2] G4: [*3], [*4], [*5], [*6], [*7] G9: [*8], [*9], [*10], [*11] G10:H, [*12] Connectivity: 7:1 E exact RC ring/chain 17:1 E exact RC ring/chain 26:2 E exact RC ring/chain 29:1 E exact RC ring/chain 30:1 E exact RC ring/chain 49:1 E exact RC ring/chain 55:1 E exact RC ring/chain Match level : 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:Atom 24:CLASS 25:CLASS 26:CLASS 27:Atom 28:CLASS 29:CLASS 30:CLASS 34:CLASS 35:Atom 36:CLASS 37:Atom 38:CLASS 39:Atom 45:CLASS 47:CLASS 48:CLASS 49:CLASS 52:CLASS 53:CLASS 54:CLASS 55:CLASS Generic attributes : Number of Carbon Atoms : less than 7 Number of Carbon Atoms : less than 7 19: Saturation : Saturated Number of Carbon Atoms : less than 7

27:

Saturation : Unsaturated

29:

Number of Carbon Atoms: less than 7

30:

Number of Carbon Atoms : less than 7

35:

Saturation : Unsaturated

37:

Saturation : Unsaturated

39:

Saturation : Unsaturated

49:

Number of Carbon Atoms : less than 7

55:

Number of Carbon Atoms: less than 7

Element Count :
Node 19: Limited

N,N1

L1 STRUCTURE UPLOADED

 \Rightarrow s 11 sss sam

SAMPLE SEARCH INITIATED 12:52:18 FILE 'MARPAT' SAMPLE SCREEN SEARCH COMPLETED - 1448 TO ITERATE

49.2% PROCESSED 712 ITERATIONS 0 ANSWERS

65.7% PROCESSED 952 ITERATIONS 8 ANSWERS

67.7% PROCESSED 980 ITERATIONS 8 ANSWERS

69.1% PROCESSED 1000 ITERATIONS (9 INCOMPLETE) 10 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.01.07

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 26832 TO 31088 PROJECTED ANSWERS: 61 TO 517

L2 10 SEA SSS SAM L1

=> s l1 sss ful

FULL SEARCH INITIATED 12:53:53 FILE 'MARPAT'
FULL SCREEN SEARCH COMPLETED - 29062 TO ITERATE

7.2% PROCESSED 2089 ITERATIONS (1 INCOMPLETE) 1 ANSWERS

13.4% PROCESSED 3903 ITERATIONS (2 INCOMPLETE) 4 ANSWERS

19.9% PROCESSED 5774 ITERATIONS (6 INCOMPLETE) 9 ANSWERS

26.7% PROCESSED 7762 ITERATIONS (18 INCOMPLETE) 24 ANSWERS

33.1% PROCESSED 9630 ITERATIONS (25 INCOMPLETE) 33 ANSWERS

40.3% PROCESSED 11723 ITERATIONS (36 INCOMPLETE) 44 ANSWERS

44.7%	PROCESSED	12981	ITERATIONS	(44	INCOMPLETE)	52	ANSWERS
47.8%	PROCESSED	13896	ITERATIONS	(53	INCOMPLETE)	63	ANSWERS
51.9%	PROCESSED	15076	ITERATIONS	(66	INCOMPLETE)	76	ANSWERS
56.2%	PROCESSED	16327	ITERATIONS	(77	INCOMPLETE)	89	ANSWERS
60.5%	PROCESSED	17573	ITERATIONS	(91	INCOMPLETE)	103	ANSWERS
65.3%	PROCESSED	18966	ITERATIONS	(108	INCOMPLETE)	121	ANSWERS
69.9%	PROCESSED	20306	ITERATIONS	(121	INCOMPLETE)	134	ANSWERS
73.5%	PROCESSED	21366	ITERATIONS	(135	INCOMPLETE)	150	ANSWERS
76.4%	PROCESSED	22194	ITERATIONS	(146	INCOMPLETE)	162	ANSWERS
79.3%	PROCESSED	23044	ITERATIONS	(157	INCOMPLETE)	173	ANSWERS
82.4%	PROCESSED	23948	ITERATIONS	(165	INCOMPLETE)	181	ANSWERS
85.0%	PROCESSED	24709	ITERATIONS	(176	INCOMPLETE)	192	ANSWERS
86.7%	PROCESSED	25188	ITERATIONS	(185	INCOMPLETE)	201	ANSWERS
88.9%	PROCESSED	25832	ITERATIONS	(202	INCOMPLETE)	218	ANSWERS
91.0%	PROCESSED	26435	ITERATIONS	(211	INCOMPLETE)	227	ANSWERS
92.7%	PROCESSED	26945	ITERATIONS	(219	INCOMPLETE)	235	ANSWERS
94.4%	PROCESSED	27445	ITERATIONS	(225	INCOMPLETE)	241	ANSWERS
95.0%	PROCESSED	27597	ITERATIONS	(230	INCOMPLETE)	246	ANSWERS
96.1%	PROCESSED	27936	ITERATIONS	(235	INCOMPLETE)	251	ANSWERS
96.7%	PROCESSED	28091	ITERATIONS	(238	INCOMPLETE)	254	ANSWERS
97.2%	PROCESSED	28239	ITERATIONS	(239	INCOMPLETE)	255	ANSWERS
97.3%	PROCESSED	28263	ITERATIONS	(240	INCOMPLETE)	256	ANSWERS
97.5%	PROCESSED	28321	ITERATIONS	(240	INCOMPLETE)	256	ANSWERS
97.7%	PROCESSED	28408	ITERATIONS	(241	INCOMPLETE)	257	ANSWERS
98.0%	PROCESSED	28479	ITERATIONS	(243	INCOMPLETE)	259	ANSWERS
98.3%	PROCESSED	28559	ITERATIONS	(245	INCOMPLETE)	261	ANSWERS
98.4%	PROCESSED	28603	ITERATIONS	(247	INCOMPLETE)	264	ANSWERS
98.5%	PROCESSED	28616	ITERATIONS	(249	INCOMPLETE)	266	ANSWERS
98.8%	PROCESSED	28710	ITERATIONS	(251	INCOMPLETE)	268	ANSWERS
99.0%	PROCESSED	28774	ITERATIONS	(252	INCOMPLETE)	269	ANSWERS
99.1%	PROCESSED	28803	ITERATIONS	(252	INCOMPLETE)	269	ANSWERS
99.2%	PROCESSED	28816	ITERATIONS	(252	INCOMPLETE)	269	ANSWERS

```
28853 ITERATIONS ( 253 INCOMPLETE)
                                                         270 ANSWERS
99.3% PROCESSED
                                                         270 ANSWERS
                                      253 INCOMPLETE)
                 28884 ITERATIONS (
 99.4% PROCESSED
                                      253 INCOMPLETE)
                                                         270 ANSWERS
                 28893 ITERATIONS (
 99.4% PROCESSED
 99.7% PROCESSED
                 28961 ITERATIONS (
                                      253 INCOMPLETE)
                                                         270 ANSWERS
                                                         270 ANSWERS
                                      253 INCOMPLETE)
 99.7% PROCESSED
                 28977 ITERATIONS (
                                      253 INCOMPLETE)
                                                         270 ANSWERS
99.8% PROCESSED
                 28991 ITERATIONS (
                                      253 INCOMPLETE)
                                                         270 ANSWERS
                 29042 ITERATIONS (
99.9% PROCESSED
                                                         270 ANSWERS
100.0% PROCESSED 29062 ITERATIONS ( 253 INCOMPLETE)
SEARCH TIME: 00.13.13
    270 SEA SSS FUL L1
1.3
=> s 13/com
          17 L3/COM
=> d his
              STRUCTURE UPLOADED
L1
           10 S L1 SSS SAM
L2
           270 S L1 SSS FUL
L3
           17 S L3/COM
L4
Uploading E:\express6\Queries\rogers2005\metX1SX2Omar.str
  a, *3
Ак—ЖН <sup>* 7</sup>
  AR . 3
                              ·-^ 10
chain nodes :
7 8 12 13 14 15 16 17 18 19 26 27 28 29 30 34 35 36 37 38 39
45 47 48 49 52 54 55
ring nodes :
1 2 3 4 5 6
ring/chain nodes :
25 53
chain bonds :
2-13 6-25 13-15 14-15 15-16 25-26 25-53 26-45 28-29 28-30 34-35 36-37
38-39 38-52 47-48 48-49 54-55
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
2-13 6-25 13-15 14-15 15-16 25-26 25-53 26-45 28-29 28-30 34-35 36-37
38-39 38-52 47-48 48-49 54-55
normalized bonds:
1-2 1-6 2-3 3-4 4-5 5-6
```

```
G1: [*1], [*2]
G4: [*3], [*4], [*5], [*6], [*7]
G9:[*8],[*9],[*10],[*11]
G10:H, [*12]
Connectivity:
7:1 E exact RC ring/chain 17:1 E exact RC ring/chain 26:2 E exact RC ring/chain
29:1 E exact RC ring/chain 30:1 E exact RC ring/chain 49:1 E exact RC
ring/chain 55:1 E exact RC ring/chain
Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 12:CLASS

      13:CLASS
      14:CLASS
      15:CLASS
      16:CLASS
      17:CLASS
      18:CLASS
      19:Atom
      24:CLASS

      25:CLASS
      26:CLASS
      27:Atom
      28:CLASS
      29:CLASS
      30:CLASS
      34:CLASS
      35:Atom

      36:CLASS
      37:Atom
      38:CLASS
      39:Atom
      45:CLASS
      47:CLASS
      48:CLASS
      49:CLASS

      52:CLASS
      53:CLASS
      54:CLASS
      55:CLASS

Generic attributes :
7:
Number of Carbon Atoms : less than 7
17:
Number of Carbon Atoms : less than 7
19:
                       : Saturated
Saturation
26:
Number of Carbon Atoms : less than 7
Saturation
                              : Unsaturated
29:
Number of Carbon Atoms : less than 7
Number of Carbon Atoms: less than 7
                              : Unsaturated
Saturation
37:
Saturation
                             : Unsaturated
39:
Saturation
                              : Unsaturated
Number of Carbon Atoms: less than 7
Number of Carbon Atoms : less than 7
Element Count :
Node 19: Limited
     N,N1
```

L5 STRUCTURE UPLOADED

=> s 15 sss sam SAMPLE SEARCH INITIATED 13:12:58 FILE 'MARPAT' SAMPLE SCREEN SEARCH COMPLETED - 1634 TO ITERATE

61.2% PROCESSED 1000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.02

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

30443 TO 34917 0 TO

PROJECTED ANSWERS:

0 SEA SSS SAM L5

=> s 15 sss ful

FULL SEARCH INITIATED 13:13:16 FILE 'MARPAT' FULL SCREEN SEARCH COMPLETED - 33458 TO ITERATE

3 ANSWERS 77.3% PROCESSED 25864 ITERATIONS 1 INCOMPLETE) 5 ANSWERS 30243 ITERATIONS (90.4% PROCESSED 9 ANSWERS 95.9% PROCESSED 32081 ITERATIONS (5 INCOMPLETE) 11 ANSWERS 99.4% PROCESSED 33245 ITERATIONS (7 INCOMPLETE)

100.0% PROCESSED 33458 ITERATIONS (8 INCOMPLETE)

12 ANSWERS

SEARCH TIME: 00.01.14

12 SEA SSS FUL L5 L7

=> d his

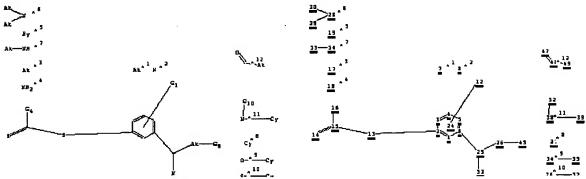
STRUCTURE UPLOADED L110 S L1 SSS SAM L2L3270 S L1 SSS FUL L417 S L3/COM L5STRUCTURE UPLOADED 0 S L5 SSS SAM L6 12 S L5 SSS FUL L7

=> s 17/com

4 L7/COM L8

=>

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chain nodes :

7 8 12 13 14 15 16 17 18 19 26 27 28 29 30 34 35 36 37 38 39 45 47 48 49 52 54 55

ring nodes :

1 2 3 4 5 6

ring/chain nodes :

25 53

chain bonds :

2-13 6-25 13-15 14-15 15-16 25-26 25-53 26-45 28-29 28-30 34-35 36-37

38-39 38-52 47-48 48-49 54-55

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

```
exact/norm bonds :
2-13 6-25 13-15 14-15 15-16 25-26 25-53 26-45 28-29 28-30 34-35 36-37
38-39 38-52 47-48 48-49 54-55
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
G1: [*1], [*2]
G4: [*3], [*4], [*5], [*6], [*7]
G9: [*8], [*9], [*10], [*11]
G10:H, [*12]
Connectivity:
7:1 E exact RC ring/chain 17:1 E exact RC ring/chain 26:2 E exact RC ring/chain
29:1 E exact RC ring/chain 30:1 E exact RC ring/chain 49:1 E exact RC
ring/chain 55:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 12:CLASS
13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:Atom 24:CLASS
25:CLASS 26:CLASS 27:Atom 28:CLASS 29:CLASS 30:CLASS 34:CLASS 35:Atom
36:CLASS 37:Atom 38:CLASS 39:Atom 45:CLASS 47:CLASS 48:CLASS 49:CLASS
52:CLASS 53:CLASS 54:CLASS 55:CLASS
Generic attributes :
Number of Carbon Atoms : less than 7
Number of Carbon Atoms: less than 7
19:
                    : Saturated
Saturation
Number of Carbon Atoms : less than 7
27:
Saturation
                     : Unsaturated
Number of Carbon Atoms : less than 7
Number of Carbon Atoms : less than 7
35:
                     : Unsaturated
Saturation
37:
                     : Unsaturated
Saturation
39:
                     : Unsaturated
Saturation
Number of Carbon Atoms : less than 7
Number of Carbon Atoms: less than 7
Element Count :
Node 19: Limited
    N,N1
```

L9 STRUCTURE UPLOADED

. `

=> s 19 sss sam
SAMPLE SEARCH INITIATED 13:17:02 FILE 'MARPAT'

80.3% PROCESSED 1000 ITERATIONS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.03

.

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

0 ANSWERS

PROJECTED ITERATIONS: 22905 TO 26895

PROJECTED ANSWERS: 0 TO

L10 0 SEA SSS SAM L9

=> s 19 sss ful

FULL SEARCH INITIATED 13:17:15 FILE 'MARPAT'

FULL SCREEN SEARCH COMPLETED - 24029 TO ITERATE

93.3% PROCESSED 22409 ITERATIONS 4 ANSWERS

99.3% PROCESSED 23870 ITERATIONS 4 ANSWERS

99.3% PROCESSED 23870 ITERATIONS 4 ANSWERS

100.0% PROCESSED 24029 ITERATIONS 4 ANSWERS

SEARCH TIME: 00.01.03

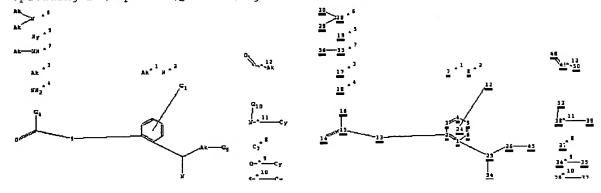
L11 4 SEA SSS FUL L9

=> s 111/com

=>

L12 4 L11/COM

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chain nodes :

7 8 12 13 14 15 16 17 18 19 26 27 28 29 30 34 35 36 37 38 39

45 48 49 50 53 55 56

ring nodes :

1 2 3 4 5 6

ring/chain nodes :

25 54

chain bonds :

1-25 2-13 13-15 14-15 15-16 25-26 25-54 26-45 28-29 28-30 34-35 36-37

38-39 38-53 48-49 49-50 55-56

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

1-25 2-13 13-15 14-15 15-16 25-26 25-54 26-45 28-29 28-30 34-35 36-37

38-39 38-53 48-49 49-50 55-56

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

```
G1:[*1],[*2]
G4: [*3], [*4], [*5], [*6], [*7]
G9: [*8], [*9], [*10], [*11]
G10:H, [*12]
Connectivity:
7:1 E exact RC ring/chain 17:1 E exact RC ring/chain 26:2 E exact RC ring/chain
29:1 E exact RC ring/chain 30:1 E exact RC ring/chain 50:1 E exact RC
ring/chain 56:1 E exact RC ring/chain
Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 12:CLASS

      13:CLASS
      14:CLASS
      15:CLASS
      16:CLASS
      17:CLASS
      18:CLASS
      19:Atom
      24:CLASS

      25:CLASS
      26:CLASS
      27:Atom
      28:CLASS
      29:CLASS
      30:CLASS
      34:CLASS
      35:Atom

      36:CLASS
      37:Atom
      38:CLASS
      39:Atom
      45:CLASS
      48:CLASS
      49:CLASS
      50:CLASS

      53:CLASS
      54:CLASS
      55:CLASS
      56:CLASS

Generic attributes :
7:
Number of Carbon Atoms : less than 7
17:
Number of Carbon Atoms : less than 7
19:
Saturation
                      : Saturated
26:
Number of Carbon Atoms: less than 7
27:
Saturation
                      : Unsaturated
29:
Number of Carbon Atoms : less than 7
Number of Carbon Atoms: less than 7
35:
                    : Unsaturated
Saturation
37:
                   : Unsaturated
Saturation
39:
Saturation
                            : Unsaturated
Number of Carbon Atoms : less than 7
Number of Carbon Atoms : less than 7
Element Count :
Node 19: Limited
    N,N1
L13 STRUCTURE UPLOADED
=> d his
L1
                     STRUCTURE UPLOADED
L2
                 10 S L1 SSS SAM
```

, •

L3

L4

L5

270 S L1 SSS FUL

STRUCTURE UPLOADED

17 S L3/COM

```
L7
           12 S L5 SSS FUL
            4 S L7/COM
L8
             STRUCTURE UPLOADED
L9
            0 S L9 SSS SAM
L10
            4 S L9 SSS FUL
L11
            4 S L11/COM
L12
              STRUCTURE UPLOADED
L13
=> s 113 sss sam
SAMPLE SEARCH INITIATED 13:20:16 FILE 'MARPAT'
SAMPLE SCREEN SEARCH COMPLETED - 1448 TO ITERATE
 52.1% PROCESSED 754 ITERATIONS
                                                          0 ANSWERS
 66.6% PROCESSED 965 ITERATIONS
                                                          6 ANSWERS
                                                          8 ANSWERS
 68.2% PROCESSED 987 ITERATIONS
 69.1% PROCESSED 1000 ITERATIONS ( 9 INCOMPLETE) 10 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.01.09
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                      BATCH **COMPLETE**
                         26832 TO 31088
PROJECTED ITERATIONS:
                             61 TO
                                     517
PROJECTED ANSWERS:
           10 SEA SSS SAM L13
=> s 113 sss sam
SAMPLE SEARCH INITIATED 13:22:04 FILE 'MARPAT'
SAMPLE SCREEN SEARCH COMPLETED - 1448 TO ITERATE
                                                          0 ANSWERS
                  716 ITERATIONS
 49.4% PROCESSED
                                                          6 ANSWERS
 64.7% PROCESSED
                  937 ITERATIONS
                                                          8 ANSWERS
                  980 ITERATIONS
 67.7% PROCESSED
                                                          9 ANSWERS
                  997 ITERATIONS
 68.9% PROCESSED
                                                        10 ANSWERS
                 1000 ITERATIONS (
                                      9 INCOMPLETE)
 69.1% PROCESSED
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.01.10
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                      BATCH **COMPLETE**
PROJECTED ITERATIONS:
                        26832 TO 31088
                             61 TO
                                       517
PROJECTED ANSWERS:
L15
            10 SEA SSS SAM L13
=> s 113 sss ful
FULL SEARCH INITIATED 13:23:43 FILE 'MARPAT'
FULL SCREEN SEARCH COMPLETED - 29062 TO ITERATE
 6.5% PROCESSED 1901 ITERATIONS (
                                      1 INCOMPLETE)
                                                         1 ANSWERS
                                                          4 ANSWERS
                                      2 INCOMPLETE)
 13.2% PROCESSED 3827 ITERATIONS (
                                      14 INCOMPLETE)
                                                         17 ANSWERS
 19.4% PROCESSED 5634 ITERATIONS (
 24.9% PROCESSED 7227 ITERATIONS ( 24 INCOMPLETE)
                                                         29 ANSWERS
```

0 S L5 SSS SAM

1.6

31.0% PROCESSED	9011 ITERATIONS	(34	INCOMPLETE)	40	ANSWERS
37.9% PROCESSED	11020 ITERATIONS	(44	INCOMPLETE)	51	ANSWERS
43.0% PROCESSED	12492 ITERATIONS	(53	INCOMPLETE)	60	ANSWERS
46.0% PROCESSED	13368 ITERATIONS	(61	INCOMPLETE)	68	ANSWERS
49.2% PROCESSED	14301 ITERATIONS	(75	INCOMPLETE)	84	ANSWERS
52.4% PROCESSED	15217 ITERATIONS	(84	INCOMPLETE)	93	ANSWERS
55.3% PROCESSED	16085 ITERATIONS	(96	INCOMPLETE)	107	ANSWERS
58.0% PROCESSED	16867 ITERATIONS	(103	INCOMPLETE)	115	ANSWERS
60.5% PROCESSED	17593 ITERATIONS	(114	INCOMPLETE)	126	ANSWERS
62.7% PROCESSED	18222 ITERATIONS	(127	INCOMPLETE)	139	ANSWERS
65.4% PROCESSED	19001 ITERATIONS	(137	INCOMPLETE)	149	ANSWERS
66.9% PROCESSED	19433 ITERATIONS	(145	INCOMPLETE)	157	ANSWERS
69.5% PROCESSED	20191 ITERATIONS	(153	INCOMPLETE)	167	ANSWERS
72.1% PROCESSED	20940 ITERATIONS	(161	INCOMPLETE)	177	ANSWERS
74.5% PROCESSED	21656 ITERATIONS	(173	INCOMPLETE)	190	ANSWERS
76.4% PROCESSED	22194 ITERATIONS	(177	INCOMPLETE)	194	ANSWERS
78.8% PROCESSED	22909 ITERATIONS	(186	INCOMPLETE)	204	ANSWERS
80.9% PROCESSED	23498 ITERATIONS	(197	INCOMPLETE)	215	ANSWERS
82.9% PROCESSED	24093 ITERATIONS	(210	INCOMPLETE)	228	ANSWERS
84.4% PROCESSED	24530 ITERATIONS	(222	INCOMPLETE)	240	ANSWERS
86.5% PROCESSED	25132 ITERATIONS	(234	INCOMPLETE)	252	ANSWERS
88.0% PROCESSED	25578 ITERATIONS	(240	INCOMPLETE)	259	ANSWERS
89.7% PROCESSED	26077 ITERATIONS	(246	INCOMPLETE)	265	ANSWERS
90.7% PROCESSED	26370 ITERATIONS	(254	INCOMPLETE)	273	ANSWERS
92.9% PROCESSED	26991 ITERATIONS	(261	INCOMPLETE)	280	ANSWERS
94.2% PROCESSED	27389 ITERATIONS	(267	INCOMPLETE)	286	ANSWERS
95.3% PROCESSED	27693 ITERATIONS	(272	INCOMPLETE)	291	ANSWERS
96.1% PROCESSED	27925 ITERATIONS	(276	INCOMPLETE)	295	ANSWERS
96.5% PROCESSED	28037 ITERATIONS	(278	INCOMPLETE)	297	ANSWERS
96.9% PROCESSED	28147 ITERATIONS	(283	INCOMPLETE)	302	ANSWERS
97.4% PROCESSED	28316 ITERATIONS	(285	INCOMPLETE)	304	ANSWERS
97.5% PROCESSED	28334 ITERATIONS	(286	INCOMPLETE)	305	ANSWERS

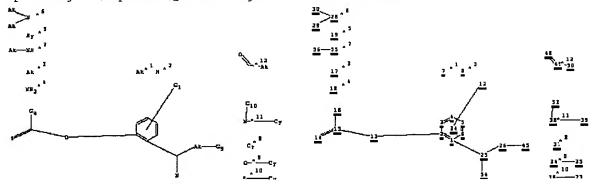
97.8%	PROCESSED	28427	ITERATIONS	(287	INCOMPLETE)	306	ANSWERS
98.0%	PROCESSED	28470	ITERATIONS	(288	INCOMPLETE)	307	ANSWERS
98.1%	PROCESSED	28499	ITERATIONS	(289	INCOMPLETE)	308	ANSWERS
98.3%	PROCESSED	28573	ITERATIONS	(292	INCOMPLETE)	311	ANSWERS
98.4%	PROCESSED	28606	ITERATIONS	(294	INCOMPLETE)	314	ANSWERS
98.6%	PROCESSED	28658	ITERATIONS	(296	INCOMPLETE)	316	ANSWERS
98.7%	PROCESSED	28687	ITERATIONS	(296	INCOMPLETE)	316	ANSWERS
98.9%	PROCESSED	28732	ITERATIONS	(297	INCOMPLETE)	317	ANSWERS
99.1%	PROCESSED	28799	ITERATIONS	(298	INCOMPLETE)	318	ANSWERS
99.1%	PROCESSED	28812	ITERATIONS	(298	INCOMPLETE)	318	ANSWERS
99.2%	PROCESSED	28816	ITERATIONS	(298	INCOMPLETE)	318	ANSWERS
99.3%	PROCESSED	28853	ITERATIONS	(299	INCOMPLETE)	319	ANSWERS
99.4%	PROCESSED	28882	ITERATIONS	(299	INCOMPLETE)	319	ANSWERS
99.4%	PROCESSED	28884	ITERATIONS	(299	INCOMPLETE)	319	ANSWERS
99.4%	PROCESSED	28901	ITERATIONS	(299	INCOMPLETE)	319	ANSWERS
99.7%	PROCESSED	28977	ITERATIONS	(299	INCOMPLETE)	319	ANSWERS
99.8%	PROCESSED	28991	ITERATIONS	(299	INCOMPLETE)	319	ANSWERS
99.9%	PROCESSED	29024	ITERATIONS	(299	INCOMPLETE)	319	ANSWERS
	PROCESSED TIME: 00.15		ITERATIONS	(299	INCOMPLETE)	319	ANSWERS

L15 319 SEA SSS FUL L13

=> s 115/com

L16 20 L15/COM

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chain nodes :
7 8 12 13 14 15 16 17 18 19 26 27 28 29 30 34 35 36 37 38 39
45 48 49 50 53 55 56
ring nodes :

```
1 2 3 4 5 6
ring/chain nodes :
25 54
chain bonds :
1-25 2-13 13-15 14-15 15-16 25-26 25-54 26-45 28-29 28-30 34-35 36-37
38-39 38-53 48-49 49-50 55-56
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-25 2-13 13-15 14-15 15-16 25-26 25-54 26-45 28-29 28-30 34-35 36-37
38-39 38-53 48-49 49-50 55-56
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
G1: [*1], [*2]
G4: [*3], [*4], [*5], [*6], [*7]
G9: [*8], [*9], [*10], [*11]
G10:H, [*12]
Connectivity:
7:1 E exact RC ring/chain 17:1 E exact RC ring/chain 26:2 E exact RC ring/chain
29:1 E exact RC ring/chain 30:1 E exact RC ring/chain 50:1 E exact RC
ring/chain 56:1 E exact RC ring/chain
Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 12:CLASS
13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:Atom 24:CLASS
25:CLASS 26:CLASS 27:Atom 28:CLASS 29:CLASS 30:CLASS 34:CLASS 35:Atom
36:CLASS 37:Atom 38:CLASS 39:Atom 45:CLASS 48:CLASS 49:CLASS 50:CLASS
53:CLASS 54:CLASS 55:CLASS 56:CLASS
Generic attributes :
Number of Carbon Atoms : less than 7
Number of Carbon Atoms : less than 7
19:
                    : Saturated
Saturation
Number of Carbon Atoms : less than 7
27:
Saturation
                     : Unsaturated
Number of Carbon Atoms : less than 7
Number of Carbon Atoms : less than 7
35:
Saturation
                     : Unsaturated
37:
Saturation
                     : Unsaturated
39:
                     : Unsaturated
Saturation
50:
Number of Carbon Atoms : less than 7
56:
Number of Carbon Atoms : less than 7
Element Count :
Node 19: Limited
   N,N1
```

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L17 STRUCTURE UPLOADED

=> s 117 sss sam

SAMPLE SEARCH INITIATED 13:40:51 FILE 'MARPAT'
SAMPLE SCREEN SEARCH COMPLETED - 1634 TO ITERATE

61.2% PROCESSED 1000 ITERATIONS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

30443 TO 34917

PROJECTED ANSWERS:

0 TO

0 ANSWERS

L18 0 SEA SSS SAM L17

=> s 117 sss ful

FULL SEARCH INITIATED 13:41:08 FILE 'MARPAT'

FULL SCREEN SEARCH COMPLETED - 33458 TO ITERATE

74.2% PROCESSED 24821 ITERATIONS 2 ANSWERS

88.6% PROCESSED 29654 ITERATIONS (4 INCOMPLETE) 7 ANSWERS

97.6% PROCESSED 32654 ITERATIONS (11 INCOMPLETE) 14 ANSWERS

98.8% PROCESSED 33053 ITERATIONS (13 INCOMPLETE) 16 ANSWERS

99.4% PROCESSED 33253 ITERATIONS (14 INCOMPLETE) 17 ANSWERS

100.0% PROCESSED 33458 ITERATIONS (15 INCOMPLETE) 18 ANSWERS

SEARCH TIME: 00.01.36

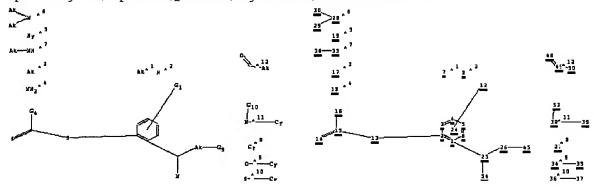
L19 18 SEA SSS FUL L17

=> s 119/com

L20 3 L19/COM

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chain nodes :

7 8 12 13 14 15 16 17 18 19 26 27 28 29 30 34 35 36 37 38 39 45 48 49 50 53 55 56

ring nodes :

1 2 3 4 5 6

ring/chain nodes :

```
25 54
chain bonds :
1-25 2-13 13-15 14-15 15-16 25-26 25-54 26-45 28-29 28-30 34-35 36-37
38-39 38-53 48-49 49-50 55-56
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-25 2-13 13-15 14-15 15-16 25-26 25-54 26-45 28-29 28-30 34-35 36-37
38-39 38-53 48-49 49-50 55-56
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
G1: [*1], [*2]
G4: [*3], [*4], [*5], [*6], [*7]
G9: [*8], [*9], [*10], [*11]
G10:H, [*12]
Connectivity:
7:1 E exact RC ring/chain 17:1 E exact RC ring/chain 26:2 E exact RC ring/chain
29:1 E exact RC ring/chain 30:1 E exact RC ring/chain 50:1 E exact RC
ring/chain 56:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 12:CLASS
13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:Atom 24:CLASS
25:CLASS 26:CLASS 27:Atom 28:CLASS 29:CLASS 30:CLASS 34:CLASS 35:Atom
36:CLASS 37:Atom 38:CLASS 39:Atom 45:CLASS 48:CLASS 49:CLASS 50:CLASS
53:CLASS 54:CLASS 55:CLASS 56:CLASS
Generic attributes :
Number of Carbon Atoms: less than 7
Number of Carbon Atoms : less than 7
19:
                     : Saturated
Saturation
Number of Carbon Atoms : less than 7
27:
                     : Unsaturated
Saturation
Number of Carbon Atoms: less than 7
Number of Carbon Atoms: less than 7
35:
Saturation
                     : Unsaturated
37:
                     : Unsaturated
Saturation
39:
Saturation
                     : Unsaturated
Number of Carbon Atoms : less than 7
Number of Carbon Atoms : less than 7
Element Count :
Node 19: Limited
```

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N,N1

L21 STRUCTURE UPLOADED

=> s 121 sss sam

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SAMPLE SEARCH INITIATED 13:44:00 FILE 'MARPAT' SAMPLE SCREEN SEARCH COMPLETED - 1245 TO ITERATE

80.3% PROCESSED 1000 ITERATIONS

0 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 2

22905 TO 26895 0 TO 0

PROJECTED ANSWERS:

L22 0 SEA SSS SAM L21

=> s 121 sss ful

FULL SEARCH INITIATED 13:44:22 FILE 'MARPAT'

FULL SCREEN SEARCH COMPLETED - 24029 TO ITERATE

84.2% PROCESSED 20236 ITERATIONS 3 ANSWERS

97.8% PROCESSED 23493 ITERATIONS 3 ANSWERS

97.8% PROCESSED 23493 ITERATIONS 3 ANSWERS

99.3% PROCESSED 23870 ITERATIONS (2 INCOMPLETE) 5 ANSWERS

100.0% PROCESSED 24029 ITERATIONS (2 INCOMPLETE) 5 ANSWERS

SEARCH TIME: 00.01.25

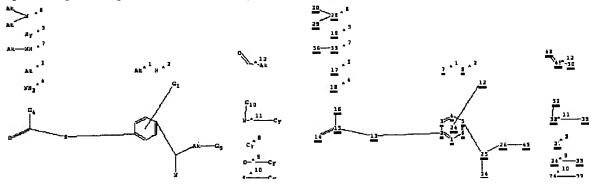
L23 5 SEA SSS FUL L21

=> s 123/com

L24 3 L23/COM

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chain nodes :

7 8 12 13 14 15 16 17 18 19 26 27 28 29 30 34 35 36 37 38 39 45 48 49 50 53 55 56

ring nodes :

1 2 3 4 5 6

ring/chain nodes :

25 54

chain bonds :

2-13 5-25 13-15 14-15 15-16 25-26 25-54 26-45 28-29 28-30 34-35 36-37 38-39 38-53 48-49 49-50 55-56

```
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
2-13 5-25 13-15 14-15 15-16 25-26 25-54 26-45 28-29 28-30 34-35 36-37
38-39 38-53 48-49 49-50 55-56
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
G1: [*1], [*2]
G4: [*3], [*4], [*5], [*6], [*7]
G9: [*8], [*9], [*10], [*11]
G10:H, [*12]
Connectivity:
7:1 E exact RC ring/chain 17:1 E exact RC ring/chain 26:2 E exact RC ring/chain
29:1 E exact RC ring/chain 30:1 E exact RC ring/chain 50:1 E exact RC
ring/chain 56:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 12:CLASS
13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:Atom 24:CLASS
25:CLASS 26:CLASS 27:Atom 28:CLASS 29:CLASS 30:CLASS 34:CLASS 35:Atom
36:CLASS 37:Atom 38:CLASS 39:Atom 45:CLASS 48:CLASS 49:CLASS 50:CLASS
53:CLASS 54:CLASS 55:CLASS 56:CLASS
Generic attributes :
7:
Number of Carbon Atoms : less than 7
17:
Number of Carbon Atoms : less than 7
19:
Saturation
                     : Saturated
Number of Carbon Atoms : less than 7
27:
                     : Unsaturated
Saturation
29:
Number of Carbon Atoms : less than 7
Number of Carbon Atoms : less than 7
35:
                     : Unsaturated
Saturation
37:
Saturation
                     : Unsaturated
39:
                      : Unsaturated
Saturation
Number of Carbon Atoms : less than 7
56:
Number of Carbon Atoms : less than 7
Element Count :
```

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=> s 125 sss sam

SAMPLE SEARCH INITIATED 13:47:25 FILE 'MARPAT'

SAMPLE SCREEN SEARCH COMPLETED - 1448 TO ITERATE

45.5% PROCESSED	659 ITERATIONS		1 ANSWERS					
61.9% PROCESSED	897 ITERATIONS		8 ANSWERS					
67.7% PROCESSED	980 ITERATIONS		17 ANSWERS					
68.2% PROCESSED	987 ITERATIONS		18 ANSWERS					
	1000 ITERATIONS (SYSTEM LIMIT EXCEEDE	20 INCOMPLETE)	21 ANSWERS					
SEARCH TIME: 00.01.17								

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 26832 TO 31088
PROJECTED ANSWERS: 277 TO 939

L26 21 SEA SSS SAM L25

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=> s 125 sss ful FULL SEARCH INITIATED 13:49:01 FILE 'MARPAT' FULL SCREEN SEARCH COMPLETED - 29062 TO ITERATE

5.0%	PROCESSED	1450	ITERATIONS	(1	INCOMPLETE)	2	ANSWERS
9.7%	PROCESSED	2829	ITERATIONS	(4	INCOMPLETE)	6	ANSWERS
11.8%	PROCESSED	3438	ITERATIONS	(12	INCOMPLETE)	17	ANSWERS
14.4%	PROCESSED	4191	ITERATIONS	(20	INCOMPLETE)	27	ANSWERS
17.1%	PROCESSED	4975	ITERATIONS	(27	INCOMPLETE)	34	ANSWERS
21.2%	PROCESSED	6160	ITERATIONS	(41	INCOMPLETE)	48	ANSWERS
24.5%	PROCESSED	7106	ITERATIONS	(51	INCOMPLETE)	58	ANSWERS
29.2%	PROCESSED	8497	ITERATIONS	(64	INCOMPLETE)	71	ANSWERS
33.8%	PROCESSED	9829	ITERATIONS	(87	INCOMPLETE)	96	ANSWERS
38.5%	PROCESSED	11182	ITERATIONS	(97	INCOMPLETE)	107	ANSWERS
42.0%	PROCESSED	12206	ITERATIONS	(107	INCOMPLETE)	117	ANSWERS
45.7%	PROCESSED	13267	ITERATIONS	(119	INCOMPLETE)	129	ANSWERS
47.5%	PROCESSED	13800	ITERATIONS	(130	INCOMPLETE)	141	ANSWERS
50.1%	PROCESSED	14555	ITERATIONS	(144	INCOMPLETE)	156	ANSWERS
51.9%	PROCESSED	15071	ITERATIONS	(154	INCOMPLETE)	166	ANSWERS
53.3%	PROCESSED	15501	ITERATIONS	(160	INCOMPLETE)	172	ANSWERS
55.4%	PROCESSED	16114	ITERATIONS	(172	INCOMPLETE)	185	ANSWERS
57.0%	PROCESSED	16560	ITERATIONS	(181	INCOMPLETE)	195	ANSWERS
58.1%	PROCESSED	16873	ITERATIONS	(187	INCOMPLETE)	202	ANSWERS

59.3%	PROCESSED	17239	ITERATIONS	(195	INCOMPLETE)	210	ANSWERS
60.9%	PROCESSED	17706	ITERATIONS	(204	INCOMPLETE)	219	ANSWERS
63.0%	PROCESSED	18320	ITERATIONS	(221	INCOMPLETE)	236	ANSWERS
65.9%	PROCESSED	19166	ITERATIONS	(229	INCOMPLETE)	244	ANSWERS
68.6%	PROCESSED	19951	ITERATIONS	(241	INCOMPLETE)	257	ANSWERS
70.9%	PROCESSED	20596	ITERATIONS	(260	INCOMPLETE)	276	ANSWERS
73.5%	PROCESSED	21366	ITERATIONS	(272	INCOMPLETE)	288	ANSWERS
75.4%	PROCESSED	21920	ITERATIONS	(279	INCOMPLETE)	296	ANSWERS
77.0%	PROCESSED	22369	ITERATIONS	(290	INCOMPLETE)	307	ANSWERS
79.2%	PROCESSED	23016	ITERATIONS	(309	INCOMPLETE)	326	ANSWERS
81.0%	PROCESSED	23532	ITERATIONS	(324	INCOMPLETE)	341	ANSWERS
82.6%	PROCESSED	24014	ITERATIONS	(336	INCOMPLETE)	353	ANSWERS
84.3%	PROCESSED	24499	ITERATIONS	(348	INCOMPLETE)	366	ANSWERS
86.2%	PROCESSED	25038	ITERATIONS	(364	INCOMPLETE)	382	ANSWERS
87.6%	PROCESSED	25465	ITERATIONS	(,	369	INCOMPLETE)	387	ANSWERS
88.8%	PROCESSED	25806	ITERATIONS	(375	INCOMPLETE)	393	ANSWERS
89.7%	PROCESSED	26066	ITERATIONS	(386	INCOMPLETE)	404	ANSWERS
90.7%	PROCESSED	26371	ITERATIONS	(391	INCOMPLETE)	409	ANSWERS
91.9%	PROCESSED	26700	ITERATIONS	(397	INCOMPLETE)	415	ANSWERS
92.8%	PROCESSED	26969	ITERATIONS	(401	INCOMPLETE)	419	ANSWERS
93.3%	PROCESSED	27128	ITERATIONS	(404	INCOMPLETE)	422	ANSWERS
94.4%	PROCESSED	27443	ITERATIONS	(408	INCOMPLETE)	426	ANSWERS
94.9%	PROCESSED	27583	ITERATIONS	(415	INCOMPLETE)	433	ANSWERS
95.6%	PROCESSED	27789	ITERATIONS	(417	INCOMPLETE)	435	ANSWERS
96.1%	PROCESSED	27941	ITERATIONS	(419	INCOMPLETE)	437	ANSWERS
96.4%	PROCESSED	28019	ITERATIONS	(422	INCOMPLETE)	440	ANSWERS
96.7%	PROCESSED	28117	ITERATIONS	(424	INCOMPLETE)	442	ANSWERS
97.1%	PROCESSED	28218	ITERATIONS	(426	INCOMPLETE)	444	ANSWERS
97.4%	PROCESSED	28303	ITERATIONS	(427	INCOMPLETE)	445	ANSWERS
97.5%	PROCESSED	28348	ITERATIONS	(429	INCOMPLETE)	447	ANSWERS
97.6%	PROCESSED	28372	ITERATIONS	(430	INCOMPLETE)	448	ANSWERS
97.7%	PROCESSED	28385	ITERATIONS	(431	INCOMPLETE)	449	ANSWERS

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97.9%	PROCESSED	28455	ITERATIONS	(433	INCOMPLETE)	451	ANSWERS
98.1%	PROCESSED	28500	ITERATIONS	(435	INCOMPLETE)	453	ANSWERS
98.2%	PROCESSED	28537	ITERATIONS	(435	INCOMPLETE)	453	ANSWERS
98.4%	PROCESSED	28587	ITERATIONS	(437	INCOMPLETE)	455	ANSWERS
98.5%	PROCESSED	28618	ITERATIONS	(439	INCOMPLETE)	457	ANSWERS
98.6%	PROCESSED	28644	ITERATIONS	(440	INCOMPLETE)	458	ANSWERS
98.7%	PROCESSED	28695	ITERATIONS	(441	INCOMPLETE)	459	ANSWERS
98.9%	PROCESSED	28743	ITERATIONS	(442	INCOMPLETE)	460	ANSWERS
99.1%	PROCESSED	28806	ITERATIONS	(444	INCOMPLETE)	462	ANSWERS
99.3%	PROCESSED	28852	ITERATIONS	(444	INCOMPLETE)	462	ANSWERS
99.4%	PROCESSED	28884	ITERATIONS	(445	INCOMPLETE)	463	ANSWERS
99.4%	PROCESSED	28890	ITERATIONS	(445	INCOMPLETE)	463	ANSWERS
99.4%	PROCESSED	28893	ITERATIONS	(445	INCOMPLETE)	463	ANSWERS
99.5%	PROCESSED	28914	ITERATIONS	(445	INCOMPLETE)	463	ANSWERS
99.6%	PROCESSED	28939	ITERATIONS	(446	INCOMPLETE)	464	ANSWERS
99.6%	PROCESSED	28939	ITERATIONS	(446	INCOMPLETE)	464	ANSWERS
99.7%	PROCESSED	28968	ITERATIONS	(446	INCOMPLETE)	464	ANSWERS
99.7%	PROCESSED	28989	ITERATIONS	(447	INCOMPLETE)	465	ANSWERS
99.8%	PROCESSED	29000	ITERATIONS	(447	INCOMPLETE)	465	ANSWERS
99.9%	PROCESSED	29024	ITERATIONS	(447	INCOMPLETE)	465	ANSWERS
99.9%	PROCESSED	29044	ITERATIONS	(447	INCOMPLETE)	465	ANSWERS
	PROCESSED TIME: 00.21		ITERATIONS	(447	INCOMPLETE)	465	ANSWERS

L27 465 SEA SSS FUL L25

=> s 127/com

L28 18 L27/COM

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```
AK* 1 , , 2
                               10
chain nodes :
7 8 12 13 14 15 16 17 18 19 26 27 28 29 30 34 35 36 37 38 39
45 48 49 50 53 55 56
ring nodes :
1 2 3 4 5 6
ring/chain nodes :
25 54
chain bonds :
2-13 5-25 13-15 14-15 15-16 25-26 25-54 26-45 28-29 28-30 34-35 36-37
38-39 38-53 48-49 49-50 55-56
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
2-13 5-25 13-15 14-15 15-16 25-26 25-54 26-45 28-29 28-30 34-35 36-37
38-39 38-53 48-49 49-50 55-56
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
G1:[*1],[*2]
G4: [*3], [*4], [*5], [*6], [*7]
G9: [*8], [*9], [*10], [*11]
G10:H, [*12]
Connectivity:
7:1 E exact RC ring/chain 17:1 E exact RC ring/chain 26:2 E exact RC ring/chain
29:1 E exact RC ring/chain 30:1 E exact RC ring/chain 50:1 E exact RC
ring/chain 56:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 12:CLASS
13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:Atom 24:CLASS
25:CLASS 26:CLASS 27:Atom 28:CLASS 29:CLASS 30:CLASS 34:CLASS 35:Atom
36:CLASS 37:Atom 38:CLASS 39:Atom 45:CLASS 48:CLASS 49:CLASS 50:CLASS
53:CLASS 54:CLASS 55:CLASS 56:CLASS
Generic attributes :
Number of Carbon Atoms: less than 7
17:
Number of Carbon Atoms : less than 7
19:
Saturation
                     : Saturated
26:
Number of Carbon Atoms : less than 7
27:
Saturation
                     : Unsaturated
29:
Number of Carbon Atoms: less than 7
30:
```

Number of Carbon Atoms: less than 7

35:

Saturation : Unsaturated

37:

Saturation : Unsaturated

39:

Saturation : Unsaturated

50:

Number of Carbon Atoms : less than 7

56:

Number of Carbon Atoms : less than 7

Element Count : Node 19: Limited

N,N1

L29 STRUCTURE UPLOADED

=> s 129 sss sam

SAMPLE SEARCH INITIATED 14:11:43 FILE 'MARPAT' SAMPLE SCREEN SEARCH COMPLETED - 1634 TO ITERATE

61.2% PROCESSED 1000 ITERATIONS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.04

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

0 ANSWERS

PROJECTED ITERATIONS: 30443 TO 34917 PROJECTED ANSWERS: 0 TO 0

L30 0 SEA SSS SAM L29

=> s 129 sss ful

FULL SEARCH INITIATED 14:12:16 FILE 'MARPAT'
FULL SCREEN SEARCH COMPLETED - 33458 TO ITERATE

66.5% PROCESSED 22260 ITERATIONS 2 ANSWERS

86.5% PROCESSED 28932 ITERATIONS 3 ANSWERS

95.3% PROCESSED 31902 ITERATIONS (8 INCOMPLETE) 11 ANSWERS

97.9% PROCESSED 32770 ITERATIONS (12 INCOMPLETE) 15 ANSWERS

99.4% PROCESSED 33253 ITERATIONS (13 INCOMPLETE) 16 ANSWERS

100.0% PROCESSED 33458 ITERATIONS (13 INCOMPLETE) 16 ANSWERS

SEARCH TIME: 00.01.27

L31 16 SEA SSS FUL L29

 \Rightarrow s 131/com

L32 3 L31/COM

=>

Uploading E:\express6\Queries\rogers2005\parX1SX2Smar.str

```
AK* H A J
                              11
                              c, *
                               10
chain nodes :
7 8 12 13 14 15 16 17 18 19 26 27 28 29 30 34 35 36 37 38 39
45 48 49 50 53 55 56
ring nodes :
1 2 3 4 5 6
ring/chain nodes :
25 54
chain bonds :
2-13 5-25 13-15 14-15 15-16 25-26 25-54 26-45 28-29 28-30 34-35 36-37
38-39 38-53 48-49 49-50 55-56
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
2-13 5-25 13-15 14-15 15-16 25-26 25-54 26-45 28-29 28-30 34-35 36-37
38-39 38-53 48-49 49-50 55-56
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
G1: [*1], [*2]
G4: [*3], [*4], [*5], [*6], [*7]
G9: [*8], [*9], [*10], [*11]
G10:H, [*12]
Connectivity:
7:1 E exact RC ring/chain 17:1 E exact RC ring/chain 26:2 E exact RC ring/chain
29:1 E exact RC ring/chain 30:1 E exact RC ring/chain 50:1 E exact RC
ring/chain 56:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 12:CLASS
13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:Atom 24:CLASS
25:CLASS 26:CLASS 27:Atom 28:CLASS 29:CLASS 30:CLASS 34:CLASS 35:Atom
36:CLASS 37:Atom 38:CLASS 39:Atom 45:CLASS 48:CLASS 49:CLASS 50:CLASS
53:CLASS 54:CLASS 55:CLASS 56:CLASS
Generic attributes :
7:
Number of Carbon Atoms : less than 7
Number of Carbon Atoms: less than 7
19:
Saturation
                     : Saturated
Number of Carbon Atoms : less than 7
Saturation
                    : Unsaturated
Number of Carbon Atoms : less than 7
```

Number of Carbon Atoms : less than 7

35:

. •

Saturation : Unsaturated

37:

: Unsaturated Saturation

: Unsaturated Saturation

Number of Carbon Atoms: less than 7

Number of Carbon Atoms: less than 7

Element Count : Node 19: Limited

N,N1

L33 STRUCTURE UPLOADED

=> s 133 sss sam

SAMPLE SEARCH INITIATED 14:14:51 FILE 'MARPAT' SAMPLE SCREEN SEARCH COMPLETED - 1245 TO ITERATE

80.3% PROCESSED 1000 ITERATIONS

0 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.06

FULL FILE PROJECTIONS: ONLINE **COMPLETE** BATCH **COMPLETE**

PROJECTED ITERATIONS: 22905 TO 26895

PROJECTED ANSWERS: 0 TO

0 SEA SSS SAM L33 T.34

=> s 133 sss ful

FULL SEARCH INITIATED 14:15:09 FILE 'MARPAT' FULL SCREEN SEARCH COMPLETED - 24029 TO ITERATE

2 ANSWERS 80.9% PROCESSED 19445 ITERATIONS

1 INCOMPLETE) 4 ANSWERS 97.8% PROCESSED 23493 ITERATIONS (

6 ANSWERS 3 INCOMPLETE) 99.3% PROCESSED 23870 ITERATIONS (

6 ANSWERS 99.3% PROCESSED 23870 ITERATIONS (3 INCOMPLETE)

99.3% PROCESSED 23870 ITERATIONS (3 INCOMPLETE) 6 ANSWERS

100.0% PROCESSED 24029 ITERATIONS (4 INCOMPLETE) 7 ANSWERS

SEARCH TIME: 00.01.35

7 SEA SSS FUL L33 L35

=> s 135/com

L36 3 L35/COM

=> d his

STRUCTURE UPLOADED L1

10 S L1 SSS SAM L2

```
L3
           270 S L1 SSS FUL
            17 S L3/COM
L5
               STRUCTURE UPLOADED
             0 S L5 SSS SAM
L6
            12 S L5 SSS FUL
L7
L8
             4 S L7/COM
ь9
              STRUCTURE UPLOADED
             0 S L9 SSS SAM
L10
L11
             4 S L9 SSS FUL
             4 S L11/COM
L12
               STRUCTURE UPLOADED
L13
            10 S L13 SSS SAM
L14
           319 S L13 SSS FUL
L15
L16
            20 S L15/COM
L17
               STRUCTURE UPLOADED
             0 S L17 SSS SAM
L18
            18 S L17 SSS FUL
L19
            3 S L19/COM
L20
              STRUCTURE UPLOADED
L21
             0 S L21 SSS SAM
L22
            5 S L21 SSS FUL
L23
L24
             3 S L23/COM
L25
               STRUCTURE UPLOADED
L26
            21 S L25 SSS SAM
L27
           465 S L25 SSS FUL
            18 S L27/COM
L28
L29
              STRUCTURE UPLOADED
L30
             0 S L29 SSS SAM
            16 S L29 SSS FUL
L31
            3 S L31/COM
L32
               STRUCTURE UPLOADED
L33
             0 S L33 SSS SAM
L34
L35
             7 S L33 SSS FUL
L36
             3 S L35/COM
=> s 14 or 18 or 112 or 116 or 120 or 124 or 128 or 132 or 136
           25 L4 OR L8 OR L12 OR L16 OR L20 OR L24 OR L28 OR L32 OR L36
=> d bib fhit 1-
L37 ANSWER 1 OF 25 MARPAT COPYRIGHT 2005 ACS on STN
    142:279952 MARPAT Full-text
     Preparation of aralkanoates as inhibitors of prostaglandin and leukotriene
     production.
    Shoda, Motoshi; Kuriyama, Hiroshi
IN
    Asahi Kasei Pharma Corporation, Japan
PA
    PCT Int. Appl., 687 pp.
SO
     CODEN: PIXXD2
DΤ
     Patent
    English
LA
FAN.CNT 4
     PATENT NO.
                   KIND DATE
                                        APPLICATION NO. DATE
     _____
                                        WO 2004-JP11952 20040813
                    A1 20050224
     WO 2005016862
PI
        W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
            CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
            GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
            LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
            NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
            TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
        RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
            AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
            EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
            SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
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SN, TD, TG
                            20050224
                                           WO 2004-XA11952 20040813
     WO 2005016862
                       A1
            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NA, NI, NO,
             NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ,
             TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
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             BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
             ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,
             SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,
             TD, TG
                                           WO 2004-XB11952 20040813
     WO 2005016862
                            20050224
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             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NA, NI, NO,
             NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ,
             TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, AM, AZ,
             BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
             ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,
             SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,
             TD, TG
    WO 2005016862
                            20050224
                                           WO 2004-XC11952 20040813
                       Α1
            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NA, NI, NO,
             NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ,
             TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM,
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, AM, AZ,
             BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
             ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,
             SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,
             TD, TG
PRAI JP 2003-293590
                      20030814
     US 2003-495734P
                      20030818
    WO 2004-JP11952
                     20040813
```

MSTR 1

G1 = Cy<EC (0-4) Q (0-) N (0-) O (0-) S (0) OTHERQ, RC (2)> (SO G34) / Cl / Br / I / OSO2Me / 64 / arylsulfonyloxy / (EX benzothienyl / benzofuranyl / naphthyl / indazolyl / indolyl / benzothiazolyl / quinolinyl / isoquinolinyl / benzotriazolyl / 111 / benzoxazolyl / 120 / 137 / 147 / 157 / 166 / 170 / 187 / 197 / 207 / 216 / 227 / 238 / 247 / 256 / 265 / 276 / 286)

```
694-C(0)-G5
       = Ak < (1-3) > / (SC G44)
       = OH / 331
G5
 39<del>1--</del>G37
G6
       = H / alkyl < (1-4) > / F / Cl / Br / NO2 / OH (SO) /
         70 / NH2 / 75 / 76 / Hy<EC (3-6) A (1-) N, AN (1) N>
         (SO alkyl<(1-4)>) / morpholino / G7 / 106 / 108
         4½—G10 76N—G10
                                           168—G35
                                1860)—G7
G7
       = alkyl<(3-8)> / 293 / Cy<EC (0-) N (0-) O (0-) S,
         RC (1-2) > / 295 / 297 / 301 / 309
 2G15-G16 2G17-G18 2G20-G18 3G17-G20-G18 3G22-G23
       = 0 / S / S(0) / S02 / 322
G8
 3½<del>2</del>—G35
       = alkyl<(1-4)> / Ph / CH2Ph
G9
       = alkyl < (1-4) > / 77 / 79
G10
 79(0)-G11 028----G12
G11
       = H / alkyl < (1-4) > / alkoxy < (1-4) > / OPh / OCH2Ph /
         NH2 / alkylamino<(1-4)> / dialkylamino<(1-4)> /
         Hy<EC (3-6) A (1-) N, AN (1) N> / morpholino
G12
       = alkyl<(1-4)> / NH2 / alkylamino<(1-4)> /
         dialkylamino<(1-4)>
       = 0 / S
G13
       = O / S / NMe
G14
       = alkylene<EC (1-3) C, DC (0) M3>
G15
       = Cb < (3-8) > (SO alkyl < (1-4) >)
G16
       = alkylene<(1-3)>(SO G19) / G15
G17
       = Cy < EC (0-) N (0-) O (0-) S, RC (1-2) >
G18
       = alkyl<(1-4)> / Ph
G19
G20
       = 0 / S / S(0) / SO2 / NH / 299
 2 N g -- G 2 1
G21
       = alkyl<(1-4)>
       = alkylene<EC (2-4) C, DC (0) M3>
G22
       = NH2 / 307
G23
```

3647-G24

= 313 / 317 G24 025—G29 G28 313 G29 = alkylene<EC (1-2) C, DC (0) M3> G25 = Cy<RC (1-2)> / H / alkyl<(1-8)>= NH / 308G27 3 8 G 3 3 G28 = 0 / s= Cy<RC (1-2)> / alkyl<(1-8)> / 315 / 320 / OH (SO) / G29 SH (SO) / NH2 (SO) / Hy<EC (1-) N, AN (1) N> / morpholino H₃C₅—G₃₀ 3C₃1—G₃₂ = Cy<RC (1-2)> G30 = alkylene<EC (1-3) C, DC (0) M3> G31 = OH / alkoxy<(1-4)> / CO2H / dialkylaminocarbonyl<(1-4)> = Cy<RC (1-2) > / alkyl<(1-8) > / 311G33 3**G2**5—G26 = R / (EX Me)G34 = G7 / Me / Et / G24 / alkyl < (1-8) > / Ph / <math>CH2PhG35 = alkyl<(1-4)> / F / Cl / Br / NO2 / OH (SO) / 329 / G36 NH2 / 325 / 328 / Hy<EC (3-6) A (1-) N, AN (1) N> / morpholino G37 = alkyl < (1-4) > / 333 / 3383G38-G39 338 C C (O) -G42-G43

G38 = alkylene<EC (2-3) C, DC (0) M3> G39 = 337 / Hy<EC (3-6) A (1-) N, AN (1) N> / morpholino

```
33 N --- G40
```

G40 = Me / Et / Pr-n G41 = H / Me / Et / Pr-n

G42 = NULL / O

G43 = alkyl<(1-4)> / cycloalkyl<(3-6)> / Ph

G44 = (1-3) CH2MPL: claim 1

NTE: additional substitution also claimed NTE: additional ring formation also claimed NTE: and protected derivatives and salts

NTE: also incorporates claim 29

RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L37 ANSWER 2 OF 25 MARPAT COPYRIGHT 2005 ACS on STN

AN 141:366254 MARPAT Full-text

TI Preparation of novel triazine compounds for inhibiting smooth muscle cell proliferation

IN Timmer, Richard T.; Alexander, Christopher W.; Pillarisetti, Sivaram; Saxena, Uday; Yeleswarapu, Koteswar Rao; Pal, Manojit; Reddy, Jangalgar Tirupathy; Krishma, Reddy Velagala Venkata Rama Murali; Sesila, Sridevi Bhatlapenumarthy; Kumar, Potlapally Rajender; Reddy, Gaddam Om

PA USA

SO U.S. Pat. Appl. Publ., 422 pp. CODEN: USXXCO

DT Patent

LA English

FAN.CNT 5

	PATENT NO.		KIND DATE		AP	PLICATION NO.	DATE	
PI	US	2004209882	A1	20041021	US	2003-400169	20030326	
	US	2005124619	A1	20050609	US	2004-951120	20040927	
PRAI	US	2001-324147P	20010	921				
	US	2002-253388	20020	923				
	US	2003-390485	20030317					
	US	2003-400169	20030	326				

MSTR 1

G1 = 0 / 178 / 180-1 181-9

1 4 8 G10 186-1810

28---G10

G3 =
$$25 / \text{Cy} < \text{EC}$$
 (10) A (0-2) N (0-2) O (0) OTHERQ (7-)
C, AR (1-), BD (6-) N, RC (2), RS (2) E6> (SO G5)

$$_{8}$$
Q---G17-C(0)-G10 $_{9}$ Q-- $_{9}$ Q(0)-G19--- $_{9}$ G21 $_{1}$ Q $_{1}$ ---G20 $_{1}$ G31

$$G6 = Li / Na / K / Mg / Ca$$

G7 =
$$C(0)$$
 / $S02$
G8 = O / S / 62

$$G8 = O / S / 62$$

$$G11 = H / alkyl < (1-10) >$$

$$G12 = Ph / OH / NH2$$

= OH / SH G13

$$G20 = (0-6) 108-101 110-103$$

$$^{\text{H}_{2}}$$
 $^{\text{C}}_{8}$ $^{\text{C}}$ $^{\text{H}_{2}}$ $^{\text{T}_{0}}$

$$186$$
 G10 142 H N 133 H N 142 H

G28 = (1-3) CH2

G29 = 184 / 187 / 194 / 199 / 232 / 237 / 244 / 251 / 258 / 263 / 268 / 271 / 278 / 284 / 290 / 301 / 310 / 318 / 369 / 378 / 438 / Ph / cyclopentyl / cyclohexyl / cycloheptyl

G30 = alkylene (SO G10) / G28 G31 =
$$202$$
 / O / S / 204

$$G32 = 0 / 206$$

286-G34

••

$$G36 = (1-2) CH2$$

 $G37 = N / CH$

$$G38 = 357 / 362$$

$$G39 = 0 / 374$$

$$G41 = C1 / Br / I / 392 / 399 / 406$$

$$_{3}9_{2}$$
—C(0)—CH2—CH2—C(0)—G47 $_{3}9_{9}$ —C(0)—CH——CH——C(0)—G47

$$G42 = R / COMe$$

$$4^{\frac{1}{9}}$$
 C(0)—CH2—CH2—C(0)—G47 $4^{\frac{1}{2}}$ C(0)—CH—CH—C(0)—G47 $4^{\frac{1}{3}}$ —

$$G44 = CH / N$$

$$G45 = O / 442 / S / SO2 / 444$$

$$G47 = OH (SO)$$

$$G48 = alkyl < (1-10) >$$

$$G49 = H / 446$$

```
G50
    = CO2H / 451
 4512-G53
G51
       = cyclohexyl / Ph
      = alkylene<EC (1-6) C, DC (0) M3> (SO)
G52
      = NH2 (SO)
G53
      = 382 / 410
G54
         H----G41
G55
     = OH / R / H
      = H / R
G56
G57
      = C(O) / alkylene<EC (1-6) C, DC (0) M3> (SO)
      = NH2 (SO) / 470 / 479
G58
G59
      = alkylene<EC (1-3) C, DC (0) M3> (SO G10) / G28
G60
      = H / NH2 (SO)
G61
      = (0-6) 498-503 500-508
 H268-CH2-580
      = (0-6) 498-495 500-497
G62
 H2CH2-500
MPL:
        claim 1
NTE:
        substitution is restricted
NTE:
        additional derivatization also claimed
L37 ANSWER 3 OF 25 MARPAT COPYRIGHT 2005 ACS on STN
    141:106367 MARPAT Full-text
    Preparation of substituted tricyclic gamma-carbolines as serotonin
    receptor agonists and antagonists
IN
    Lee, Taekyu; Chen, Wenting; Deng, Wei; Robichaud, Albert; Wexler, Ruth
    Bristol-Myers Squibb Company, USA
PA
so
    PCT Int. Appl., 256 pp.
    CODEN: PIXXD2
DT
    Patent
LA
    English
FAN.CNT 1
                     KIND DATE
    PATENT NO.
                                         APPLICATION NO. DATE
                     ____
                                          _____
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20040708

A2

WO 2004056324

PΙ

WO 2003-US41447 20031219

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WO 2004056324
                      A3 20040902
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO,
             NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ,
             TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
             BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
             ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,
             TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     US 2004180875
                       A1 20040916
                                           US 2003-743449 20031219
PRAI US 2002-434760P 20021219
  MSTR 1
G1
       = H / CHO / 15 / 18 / 23 / 20 / cycloalkyl<(3-6)> /
         Ak < EC (1-) C, BD (0-) D (0-) T > (SO (1-) G4) /
         aryl<(6-10)> (SO) / Cb<(3-10)> (SO) /
         Hy<EC (5-6) A (1-4) Q (0-) N (0-) O (0-) S (0) OTHERQ,
         RC (1), RS (1) M5 (1) X6> (SO) / 27 / (SC Me / Et)
               О
1 — ОН 2 G3 — G2 2 S — ОН
G2
       = alkyl < (1-4) > (SO (1-) aryl < (6-10) >) /
         alkyl<(1-4)> (SR cycloalkyl<(3-6)>)
G3
       = C(0) / S(0) / S02
       = F / Cl / Br / I / alkoxy<(1-4)> /
G4
         cycloalkyl<(3-6)> / aryl<(6-10)> (SO) / Cb<(3-10)> (SO) /
         Hy<EC (5-6) A (1-4) Q (0-) N (0-) O (0-) S (0) OTHERQ,
         RC (1), RS (1) M5 (1) X6> (SO) / 25
 285=0
G5
       = Cb < (3-10) > (SO) / Hy < EC (5-6) A (1-4) Q (0-) N (0-)
         O (0-) S (0) OTHERQ, RC (1), RS (1) M5 (1) X6> (SO)
G6
       = (1-2) 33
 ዟና----G7
G7
      = H / alkyl<(1-4)>
      = H / alkyl < (1-4) > (SO (1-2) G10) /
G8
        alkylcarbonyl<(1-4)> / alkoxycarbonyl<(1-4)> /
         alkyl < (1-4) > (SR (1-) G9) / (SC Me / Et)
      = F / Cl / Br / I
G9
      = F / Cl / Br / I / OH / CF3 / CN / NO2 / CO2H /
G10
```

```
alkylthio<(1-4)> / 36 / 41 / 44 / NH2 /
          alkyl < (1-4) > (SO (1-) G9) / alkenyl < (2-6) > / alkynyl < (2-6) > /
          alkoxy<(1-4)> / Cb<(3-10)> (SO) / aryl<(6-10)> (SO) /
          Hy<EC (5-10) A (1-4) Q (0-) N (0-) O (0-) S (0) OTHERQ>
          (SO) / 46
  _{3}^{G11}-S02-G12 _{4}^{G11}-C(0)-G12 _{4}^{G11}-G13 _{4}^{G14}=0
G11
       = NH / 39
 3 N ----- G12
G12
        = alkyl<(1-4)>
G13
        = alkyl<(1-4)> / alkylaminocarbonyl<(1-4)> /
          alkylsulfonyl<(1-4)> / alkoxycarbonyl<(1-4)> /
          alkylcarbonyl<(1-4)> / CHO
G14
        = Cb < (3-10) > (SO) / Hy < EC (5-10) A (1-4) Q (0-) N (0-)
          O(0-) S(0) OTHERQ> (SO)
G15
        = F / Cl / Br / I / CF3 / OCF3 / CN / NO2 / OMe /
          SMe / 49 / 51 / 59 / 62 / 65 / 66 / 71 /
          Hy \le C (5-6) A (1-) N (0-) O (0) OTHERQ, AN (1-) N, RC (1),
          RS (1) M5 (1) X6> (SO alkyl<(1-4)>') /
          Hy<EC (9-10) A (1-4) Q (1-) N (0-) O (0-) S (0) OTHERQ,
          AN (1-) N, RC (2) > (SO) / 74 / alkyl<(1-4) > (SR (1-) G9) /
          alkoxy<(1-4)> (SR (1-) G9) / Ak<EC (1-) C, BD (0-) D (0-) T>
          (SO) / Cb<(3-6)> (SO) / 76 / (SC OEt / SEt / S(O)Me / SO2Me /
          Me / Et / Pr-n / Pr-i / Bu-n / Bu-i / Bu-s)
 F_{4}§——CF3 _{5}G17—G16 _{5}9——CF2—CF3 _{6}2——CF2—H _{6}9——CF2—Me
 6 G 1 9 - G 1 8 - G 1 6 H 2 C - G 1 7 - G 1 6 7 G 2 0 - G 2 1 7 G 2 2 = O
G16
       = Ak<(1-)> (SO) / Cb<(3-10)> (SO) /
          aryl<(6-10)>(SO) / Hy<EC (5-10) A (1-4) Q (0-) N (0-) O (0-)
         S (0) OTHERQ> (SO) / 53
 5914=0
    = 0 / S / S(0) / SO2 / NH / 55
 5 § ----- G12
       = NH / 69
G18
 6 N ---- G12
G19
     = S(0) / SO2 / C(0)
```

alkylsulfonyl<(1-4)> / alkylsulfinyl<(1-4)> /

```
G20
       = S(0) / SO2. / CH2 / C(0)
G21
       = Hy<EC (5-6) A (1-) N (0-) O (0) OTHERQ, AN (1-) N,
         RC (1), RS (1) M5 (1) X6> (SO alkyl<(1-4)>) /
         Hy<EC (9-10) A (1-4) Q (1-) N (0-) O (0-) S (0) OTHERQ,
         AN (1-) N, RC (2) > (SO)
G22
       = Cb < (3-6) > (SO)
G23
       = (1) G25 / (-2) G24 / (-2) H
G24
       = F / Cl / Br / CF3 / OCF3 / OH / CN / NO2 / 81 /
         alkyl < (1-4) > (SO (1-) G9) / alkenyl < (2-4) > / alkynyl < (2-4) > /
         alkoxy<(1-4)>(SO(1-)G9)
 F2C----CF3
G25
       = F / Cl / Br / I / CF3 / OCF3 / OH / CN / NO2 / OMe /
         SMe / 83 / OH / SH / NH2 / 85 /
         Hy < EC (5-6) A (1-) N (0-) O (0) OTHERQ, AN (1-) N, RC (1),
         RS (1) M5 (1) X6> (SO alkyl<(1-4)>) /
         Hy<EC (9-10) A (1-4) Q (1-) N (0-) O (0-) S (0) OTHERQ,
         AN (1-) N, RC (2) > (SO) / 91 / 93 / 99 / 106 / 111 / 113 /
         116 / 122 / 133 / Ak<EC (1-) C, BD (0-) D (0-) T>
         (SO (1-) G43) / cycloalkyl < (3-6) > (SO (1-) G44) /
         Cb < (3-10) > (SO (1-) G45)
 F23-CF3 8526-G46 95(0)-G46 95(0)-G30 9532-C(0)-G33 186-C(0)-G34
 111 OH
               _ОН
                     1635-G36 1638-G39 1640-G41
       = 0 / S / NH / 87 / S(0) / SO2
 8 N ---- G28
G27
       = Ak < EC (1-) C, BD (0-) D (0-) T > (SO) / 89 /
         cycloalkyl<(3-6)>(SO) / aryl<(6-10)>(SO) /
         Cb < (3-10) > (SO) / Hy < EC (5-10) A (1-4) Q (0-) N (0-) O (0-)
         S (0) OTHERQ> (SO)
 8<sup>6</sup>29=0
G28
       = alkyl<(1-4)> / alkenyl<(2-4)> / alkynyl<(2-4)>
G29
       = Ak < EC (1-) C, BD (0-) D (0-) T > (SO)
       = NH2 / 95 / Hy<EC (5-6) A (1-) N (0-) O (0) OTHERQ,
G30
         AN (1-) N, RC (1), RS (1) M5 (1) X6> (SO alkyl<(1-4)>) /
         Hy<EC (9-10) A (1-4) Q (1-) N (0-) O (0-) S (0) OTHERQ,
         AN (1-) N, RC (2) > (SO) / OH
9631-G27
```

```
G32
       = NH / 102 / 0
 1 <del>0 2 G</del>12
G33
       = H / Ak < EC (1-) C, BD (0-) D (0-) T > (SO) / 104 /
        S (0) OTHERQ> (SO)
 1649=0
G34
      = OH / 109
 18<del>9 G</del>27
G35
       = S(0) / S02
G36
       = NH2 / 118 / Hy<EC (5-6) A (1-) N (0-) O (0) OTHERQ,
        AN (1-) N, RC (1), RS (1) M5 (1) X6> (SO\ alkyl < (1-4) >) /
        Hy<EC (9-10) A (1-4) Q (1-) N (0-) O (0-) S (0) OTHERQ,
        AN (1-) N, RC (2) > (SO)
 1937-G27
G37
    = NH / 120 / (SC NMe / NEt)
 1 ½ 0 G28
    = NH / 124
G38
 1 2 4 G12
G39
    = 126 / 128 / 131
                  1935—G27
              -0H
G40
     = NH / 135
135 G27
```

= CHO / CO2H / 137 / CONH2 / 140 / 142 / 145

Çē

9 N ----- G 2 8

G41

0 137 OH 1660)-G28 1660)-G42-G28 0645-G28

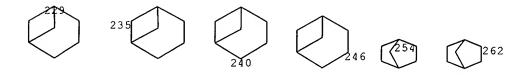
G42 = O / NH

G43 = R / (SC OH / OMe / OEt / OPr-n / OPr-i / F / OCF3 / CN / NO2 / SMe / SEt / SO2Me / NH2 / NHMe / NMe2 / COMe / CO2Me / NHCOMe / CONH2 / CHO / Ph (SO) / pyridyl (SO))

G44 = R / (SC F / Cl / Br / Me / Et / Pr-n / Pr-i / Bu-n / Bu-i / Bu-s / Bu-t / OH / OMe / OEt / OPr-n / OPr-i / CF3 / OCF3 / CN / NO2 / 147 / SMe / SEt / SO2Me / NH2 / 149 / 152 / NHMe / NMe2 / COMe / CO2Me / NHCOMe / CONH2 / CHO / CH(OH)Me / CH2OH / CH2CH2OH / CH2OMe / 156 / 159 / Ph (SO) / pyridyl (SO))

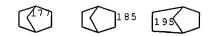
G45 = R / (SC F / Cl / Br / Me / Et / Pr-n / Pr-i / Bu-n / Bu-i / Bu-s / Bu-t / OH / OMe / OEt / OPr-n / OPr-i / CF3 / OCF3 / CN / NO2 / 161 / SMe / SEt / SO2Me / NH2 / 163 / 166 / NHMe / NMe2 / COMe / CO2Me / NHCOMe / CONH2 / CHO / CH(OH)Me / CH2OH / CH2CH2OH / CH2OMe / 170 / 173)

G46 = Ak<EC (1-) C, BD (0-) D (0-) T> (SO (1-) G47) / 273 / cycloalkyl<(3-6)> (SO (1-) G45) / aryl<(6-10)> (SO (1-) G45) / Cb<(3-10)> (SO (1-) G45) / Hy<EC (5-10) A (1-4) Q (0-) N (0-) O (0-) S (0) OTHERQ> (SO (1-) G45) / (SC cyclopropyl / cyclobutyl / cyclopentyl / cyclohexyl / 229 / 235 / 240 / 246 / 254 / 262 / 272 / Ph / pyridyl / Me / Et / Pr-n / Bu-n / pentyl / hexyl)



29390

G47 = R / (SC F / Cl / OH / cyclopropyl / cyclobutyl / cyclopentyl / cyclohexyl / 177 / 185 / 195 / 201 / 207 / 212 / 218 / Ph)







MPL: claim 1

NTE: or pharmaceutically acceptable salts

NTE: substitution is restricted

STE: or stereoisomers

L37 ANSWER 4 OF 25 MARPAT COPYRIGHT 2005 ACS on STN

AN 140:315087 MARPAT Full-text

TI Pharmaceuticals containing (hydroxybenzyl) amines as acetylcholine esterase inhibitors and selective serotonin reuptake inhibitors

IN Koyama, Kazuo; Marumoto, Masashi; Toda, Seihiro; Suzuki, Keiko; Furumoto, Hiroshi

PA BTG International Ltd., UK

SO Jpn. Kokai Tokkyo Koho, 141 pp. CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2004107322	A2	20040408	JP 2003-200434	20030723
PRAI	JP 2002-214641	20020724			

MSTR 1

G1 = alkyl<(1-6)> / NH2 / alkylamino<(1-6)> /
dialkylamino<(1-6)> / Hy<EC (1-4) Q (1-) N (0-) O (0-) S (0)
OTHERQ, BD (ALL) SE, RS (0-) E5 (0-) E6 (0-) E7 (0) OTHER> /
(SC 19) / (EX morpholino)

G2 = 13-3 14-6 / 16 / (EX 63-3 70-6)

G3 = aryl<(-14)> (SO (1-3) G4) /
heteroaryl<EC (5-10) A (1-3) Q (0-) N (0-) O (0-) S (0)
OTHERQ> (SO (1-3) G4) / (SC Ph (SO (1-3) G18) /
pyridyl (SO (-1) G4) / 35 / 43) / (EX 49 / naphthyl / 57)

G4 = F / Cl / Br / I / alkyl<(1-6)> (SO (1-) G5) / alkoxy<(1-6)> / alkylthio<(1-6)> / CHO / alkylcarbonyl<(1-6)> / alkoxycarbonyl<(1-6)> / NH2 / NHCHO / alkylcarbonylamino<(1-6)> / OH / SH / CN / NO2 / CO2H

G5 = F / Cl / Br / I

G6 = alkylene<(1-6)> / 9-4 10-7 / (SC CH2 / CH2CH2)

G7 = alkylene
$$<(1-6)>$$
 / (SC CH2 / CH2CH2)
G8 = O / S / NH / 11

1⅓——G9

G9 = CHO / alkylcarbonyl<
$$(1-6)$$
>

G10 = phenylene

G12 = NH2 / 22 / 24

G13 =
$$Hy < EC$$
 (1) N (8-10) C, AN (1) N, BD (60) D, RC (2-), RS (1-) E6>

G14 = H / alkyl < (1-6) > / (SC Me / Et)

G15 = 0 / S

G16 = Me / Et

G17 = alkyl<(1-6)> / (SC Me / Et)

```
= alkylene<(1-3)> / (SC CH2 / CH2CH2)
G19
       = G22 / 72-65 74-69
 ₩<u>Ç</u>——CH———ÇH2
G21
       = H / Me
G22
       = (1-3) CH2
       = alkylene<(1-3)> / (SC CH2 / CH2CH2)
        claim 1
NTE:
        additional ring formation also claimed
NTE:
        or pharmacologically acceptable salts or esters
L37 ANSWER 5 OF 25 MARPAT COPYRIGHT 2005 ACS on STN
     139:268384 MARPAT Full-text
AN
     Preparation of quaterphenyls and related compounds via combinatorial
ΤI
     chemistry for use as liquid crystals
IN
     Pauluth, Detlef; Kirsch, Peer; Baeuerle, Peter; Deeg, Oliver
PA
     Merck Patent G.m.b.H., Germany
     Eur. Pat. Appl., 48 pp.
     CODEN: EPXXDW
DT
     Patent
LA
    German
FAN.CNT 1
     PATENT NO.
                                       APPLICATION NO. DATE
                    KIND DATE
                    ----
                                        -----
     -----
    EP 1346995 A1 20030924 EP 2003-3811 20030220
PΙ
        R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
     DE 10211597
                   A1 20031002 DE 2002-10211597 20020315
     JP 2003286208
                    A2 20031010
                                       JP 2003-69260
     US 2004006235 A1 20040108
                                       US 2003-388607 20030317
PRAI DE 2002-10211597 20020315
  MSTR 1
 G9-G1-G10-G8-G9
G1
      = NULL / p-C6H4 (SO (1-) G2) /
        Hy<EC (6) A (1-2) N (4-5) C (0) OTHERQ, AR (1-),
        AN (0) N (2-) C, BD (ALL) N, RC (1), RS (1) E6> (SO (1-) G2)
G2
      = alkyl<(1-12)> / alkenyl<(2-12)> / 7 /
        Ph (SO alkyl<(1-12)>) / F / Cl / Br / I / OH / SH / 9 / CN /
        NO2 / 14 / CF3 / NH2 / 22
         §4—G5 1¾==0 2€7—G5
      = H / Ak < (1-11) > (SO) / R / OH / 18 / NH2
G3
186--G5
G4
      = 0 / s
G5
      = alkyl<(1-12)> / alkenyl<(2-12)> / 12 /
```

G6 = O / NH / 20

2N----G5

G7 = NH / 24

2Ŋ——G5

- G8 = p-C6H4 / Cb<EC (6) C, AR (1-), BD (ALL) N, RC (1), RS (1) E6> (SO (1-) G2) / Hy<EC (6) A (1-2) N (4-5) C (0) OTHERQ, AR (1-), AN (0) N (2-) C, BD (ALL) N, RC (1), RS (1) E6> (SO (1-) G2)
- G9 = H / F / Cl / CN / NCS / alkyl<(1-12)> (SO (1-) F) / alkoxy<(1-12)> (SO (1-) F) / alkenyl<(2-8)> (SO (1-) F) / alkynyl<(2-8)> (SO (1-) F)
- G10 = 26-2 28-4 / 29-2 30-4 / 31-2 42-4 / 53-2 64-4 / 75-2 86-4 / Hy<EC (13-14) A (1-2) N (11-13) C (0) OTHERQ, AN (0) N, AR (1-), BD (12) N (-1) D, FA (4) C (0) N, RC (3), RS (-1) E5 (-3) E6 (0) OTHER> (SO (1-) G2)

$$2^{G11-G13} - 2^{G12} - 2^{G15} - 3^{G16}$$

$$G17 \qquad G17 \qquad G$$

- G11 = p-C6H4 / Cb<EC (6) C, AR (1-), BD (ALL) N, RC (1), RS (1) E6> (SO (1-) G2) / Hy<EC (6) A (1-2) N (4-5) C (0) OTHERQ, AR (1-), AN (0) N (2-) C, BD (ALL) N, RC (1), RS (1) E6> (SO (1-) G2)
- G12 = p-C6H4 / Cb<EC (6) C, AR (1-), BD (ALL) N, RC (1), RS (1) E6> (SO (1-) G2) / Hy<EC (6) A (1-2) N (4-5) C (0) OTHERQ, AR (1-), AN (0) N (2-) C, BD (ALL) N, RC (1), RS (1) E6> (SO (1-) G2)
- G13 = CH2CH2 / CH=CH / ethynylene / p-C6H4 /
 Cb<EC (6) C, AR (1-), BD (ALL) N, RC (1), RS (1) E6>
 (SO (1-) G2) / Hy<EC (6) A (1-2) N (4-5) C (0) OTHERQ,
 AR (1-), AN (0) N (2-) C, BD (ALL) N, RC (1), RS (1) E6>
 (SO (1-) G2)
- G14 = H / Ak < (1-11) > (SO) / R
- G15 = p-C6H4 / Cb < EC (6) C, AR (1-), BD (ALL) N, RC (1),

```
RS (1) E6> (SO (1-) G2) / Hy<EC (6) A (1-2) N (4-5) C (0)
         OTHERQ, AR (1-), AN (0) N (2-) C, BD (ALL) N, RC (1),
         RS (1) E6> (SO (1-) G2)
G16
       = p-C6H4 / Cb<EC (6) C, AR (1-), BD (ALL) N, RC (1),
         RS (1) E6> (SO (1-) G2) / Hy<EC (6) A (1-2) N (4-5) C (0)
         OTHERQ, AR (1-), AN (0) N (2-) C, BD (ALL) N, RC (1),
         RS (1) E6> (SO(1-) G2)
G17
       = H / R
MPL:
         claim 1
NTE:
         additional interruptions of alkyl, alkoxy, alkenyl, and alkynyl in G9
         also claimed
NTE:
         substitution is restricted
RE.CNT 23
              THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD
              ALL CITATIONS AVAILABLE IN THE RE FORMAT
     ANSWER 6 OF 25 MARPAT COPYRIGHT 2005 ACS on STN
     139:100974 MARPAT Full-text
AN
TΙ
     Preparation of 4-dedimethylamino (substituted) tetracycline compounds for
     treating tetracycline responsive states
     Nelson, Mark L.; Ohemeng, Kwasi
IN
     Paratek Pharmaceuticals, Inc., USA
     PCT Int. Appl., 181 pp.
     CODEN: PIXXD2
DT
     Patent
LA
    English
FAN.CNT 1
     PATENT NO.
                    KIND DATE
                                           APPLICATION NO. DATE
     -----
                      ----
                                           -----
    WO 2003057169
                     A2
PΙ
                            20030717
                                           WO 2003-US336
                                                            20030106
     WO 2003057169
                      A3 20031204
        W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA,
             UG, UZ, VC, VN, YU, ZA, ZM, ZW
        RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF,
             BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
    US 2004157806
                     A1 20040812 US 2003-337914 20030106
A2 20041110 EP 2003-729351 20030106
    EP 1474380
        R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
     JP 2005514410
                      T2 20050519
                                           JP 2003-557528 20030106
PRAI US 2002-346929P
                     20020108
    US 2002-346930P
                     20020108
    US 2002-346956P 20020108
    US 2002-347065P
                     20020108
    US 2002-367049P 20020321
    WO 2003-US336
                      20030106
```

MSTR 1

..

```
28 — G30 26 <del>— G</del>37
        = Me / Ak<EC (1-) C, BD (0-) D (0-) T> (SO (1-) G3)
 G2
        = OH / Cb<BD (0-) D (0-) T> (SO G6) / F / Cl / Br /
 G3
          I / CN / SH / NH2 / 30 / Cb<EC (6-) C, AR (1-),
          BD (6-) N (0-) D, RC (1-), RS (0-) E5 (0-) E6> (SO G6) /
          Hy \le C (5-) A (1-4) Q (0-) N (0-) O (0-) S (0-) P, AR (1-),
          BD (2-) D, RC (1-), RS (0-) E5 (0-) E6> (SO G6)
 364-G5
G4
        = O / S / S(O) / SO2 / NH
G5
       = alkyl (SO) / cycloalkyl (SO)
G6
       = alkyl (SO) / cycloalkyl (SO) / R
       = H / OH / F / Cl / Br / I / SH /
          Ak < BD (0-) D (0-) T > (SO) / Cb < BD (0-) D (0-) T > (SO) /
          Cb<EC (6-) C, AR (1-), BD (6-) N (0-) D, RC (1-),
          RS (0-) E5 (0-) E6> (SO G6) / Hy<EC (5-) A (1-4) Q (0-)
          N (0-) O (0-) S (0-) P, AR (1-), BD (2-) D, RC (1-),
          RS (0-) E5 (0-) E6> (SO G6) / 32 / 34
 364---G5
         H2C-R
G8
       = NH2 / 39 / 41
       = Ak < BD (0-) D (0-) T > (SO) /
G9
         Cb < BD (0-) D (0-) T > (SO) / 44 /
         Cb<EC (6-) C, AR (1-), BD (6-) N (0-) D, RC (1-),
         RS (0-) E5 (0-) E6> (SO G6) / Hy<EC (5-) A (1-4) Q (0-)
         N (0-) O (0-) S (0-) P, AR (1-), BD (2-) D, RC (1-),
         RS (0-) E5 (0-) E6> (SO G6) / Hy<EC (0-) N (0-) O (0-) S (0-)
         P, AR (0) > (SO) / R<TX "prodrug moiety">
 4 G 4 --- G 5
G10
     = 260 / C(0)
G11
      = OH / 56
58----G12
```

G1

= 21 / 25 / 245 / S / 28 / O

```
G12
        = R<TX "prodrug moiety">
 G14
        = OH / H / SH / 63 / Cb<EC (6-) C, AR (1-),
          BD (6-) N (0-) D, RC (1-), RS (0-) E5 (0-) E6> (SO G6) /
          Hy<EC (5-) A (1-4) Q (0-) N (0-) O (0-) S (0-) P, AR (1-),
          BD (2-) D, RC (1-), RS (0-) E5 (0-) E6> (SO G6) /
          Ak < BD (0-) D (0-) T > (SO) / Cb < BD (0-) D (0-) T > (SO) / 65 /
  69(0)-G15 694-G5 69-C(0)-G17
 G15
        = Ak < BD (0-) D (0-) T> (SO (1-) G16) /
          Cb<BD (0-) D (0-) T> (SO G16) /
          Cb<EC (6-) C, AR (1-), BD (6-) N (0-) D, RC (1-),
          RS (0-) E5 (0-) E6> (SO) / Hy<EC (5-) A (1-4) Q (0-) N (0-)
          O (0-) S (0-) P, AR (1-), BD (2-) D, RC (1-),
          RS (0-) E5 (0-) E6> (SO)
        = Cb<EC (6-) C, AR (1-), BD (6-) N (0-) D, RC (1-),
 G16
          RS (0-) E5 (0-) E6> (SO) / Hy<EC (5-) A (1-4) Q (0-) N (0-)
          O (0-) S (0-) P, AR (1-), BD (2-) D, RC (1-),
          RS (0-) E5 (0-) E6> (SO)
        = Ak < BD (0-) D (0-) T > (SO) /
G17
          Cb < BD (0-) D (0-) T > (SO) / Cb < EC (6-) C, AR (1-),
          BD (6-) N (0-) D, RC (1-), RS (0-) E5 (0-) E6> (SO) /
          Hy<EC (5-) A (1-4) Q (0-) N (0-) O (0-) S (0-) P, AR (1-),
          BD (2-) D, RC (1-), RS (0-) E5 (0-) E6> (SO)
G18
        = NO2 / Ak<BD (0-) D (0-) T> (SO (1-) G42) /
          Cb<BD (0-) D (0-) T> (SO) / Cb<EC (6-) C, AR (1-),
          BD (6-) N (0-) D, RC (1-), RS (0-) E5 (0-) E6> (SO G20) /
         Hy<EC (5-) A (1-4) Q (0-) N (0-) O (0-) S (0-) P, AR (1-),
         BD (2-) D, RC (1-), RS (0-) E5 (0-) E6> (SO G20) / 71 /
         NH2 (SO) / 73 / 103 / (SC Ph (SO (1-) G29) / naphthyl (SO) /
          thiazolyl / thienyl / furyl / Me / Et / Pr-i / Pr-n / Bu-n /
         Bu-i / Bu-t / pentyl / hexyl / cyclopentyl / cyclohexyl /
         cyclopropyl / cyclobutyl / alkylcarbonyl (SO (1-) G43) /
         267 / 269 / SO2NH2 (SO) / 273 / COMe / loweralkylamino /
         diloweralkylamino)
 7G19-G5
           G22
7G21—G22—G23 1G32—G23 提展—G44 提展—C(0)-0—G45
 ₽Ŋ<del>3</del>—SO2—R
G19
       = 0 / s / s(0) / so2
       = Ak < BD (0-) D (0-) T > (SO) /
G20
         Cb < BD (0-) D (0-) T > (SO) / R
G21
       = (1-3) CH2
G22
       = 0 / NH / 77 / S
 7 N ----- G2 4
G23
       = SH / NH2 / OH / 79 / Me /
```

Ak<BD (0-) D (0-) T> (SO (1-) G25)

. •

7 622-G24

```
G24
        = acyl / Ak < BD (0-) D (0-) T > (SO) /
          Cb<BD (0-) D (0-) T> (SO) / 83 /
          Cb<EC (6-) C, AR (1-), BD (6-) N (0-) D, RC (1-),
          RS (0-) E5 (0-) E6> (SO G6) / Hy<EC (5-) A (1-4) Q (0-)
          N (0-) O (0-) S (0-) P, AR (1-), BD (2-) D, RC (1-),
          RS (0-) E5 (0-) E6> (SO G6) / Hy<EC (0-) N (0-) O (0-) S (0-)
          P, AR (0) > (SO) / R<TX "prodrug moiety" > / (SC Ph (SO))
  894-G5
 G25
        = acyl / Cb < BD (0-) D (0-) T > (SO) / 85 /
          Cb<EC (6-) C, AR (1-), BD (6-) N (0-) D, RC (1-),
          RS (0-) E5 (0-) E6> (SO G6) / Hy<EC (5-) A (1-4) Q (0-)
          N (0-) O (0-) S (0-) P, AR (1-), BD (2-) D, RC (1-),
          RS (0-) E5 (0-) E6> (SO G6) / Hy<EC (0-) N (0-) O (0-) S (0-)
          P, AR (0) > (SO) / R < TX "prodrug moiety">
 8 9 4 --- G5
G26
       = H / NO2 / Ak < BD (0-) D (0-) T > (SO G47) /
          Cb < BD (0-) D (0-) T > (SO) / Cb < EC (6-) C, AR (1-),
          BD (6-) N (0-) D, RC (1-), RS (0-) E5 (0-) E6> (SO G20) /
         Hy < EC (5-) A (1-4) Q (0-) N (0-) O (0-) S (0-) P, AR (1-),
          BD (2-) D, RC (1-), RS (0-) E5 (0-) E6> (SO G20) / 88 / NH2 /
          90 / 95 / 108 / (SC Ph (SO (1-) G46) / Me / Et / Pr-i /
          Pr-n / Bu-i / Bu-t / Bu-n / pentyl / hexyl / COMe)
 8G19-G5
G27
       = H / OH / F / Cl / Br / I / SH /
         Ak < BD (0-) D (0-) T > (SO) / Cb < BD (0-) D (0-) T > (SO) /
         Cb<EC (6-) C, AR (1-), BD (6-) N (0-) D, RC (1-),
         RS (0-) E5 (0-) E6> (SO G6) / Hy<EC (5-) A (1-4) Q (0-)
         N (0-) O (0-) S (0-) P, AR (1-), BD (2-) D, RC (1-),
         RS (0-) E5 (0-) E6> (SO G6) / 98
 964-G5
G29
       = R / (SC alkyl (SO) / NH2 (SO) / alkoxy (SO) / 263 /
         NO2 / F / Cl / Br / I / OMe)
 ₽8<del>3--</del>C(O)-O---G41
G30
       = H / OH / F / Cl / Br / I / SH /
         Ak < BD (0-) D (0-) T > (SO) / Cb < BD (0-) D (0-) T > (SO) /
         Cb<EC (6-) C, AR (1-), BD (6-) N (0-) D, RC (1-),
```

```
RS (0-) E5 (0-) E6> (SO G6) / Hy<EC (5-) A (1-4) Q (0-)
           N (0-) O (0-) S (0-) P, AR (1-), BD (2-) D, RC (1-),
           RS (0-) E5 (0-) E6> (SO G6) / 112 / 114
  _{1}G4-G5 _{1}1_{1}4-R
 G37
      = 247 / 250 / 253
  24 + \frac{G38}{G38} \quad 250 + \frac{G38}{G39} \quad 253 + \frac{G39}{G39}
 G38
        = H / OH / F / Cl / Br / I / SH /
          Cb<BD (0-) D (0-) T> (SO) / Cb<EC (6-) C, AR (1-),
          BD (6-) N (0-) D, RC (1-), RS (0-) E5 (0-) E6> (SO G6) /
          Hy<EC (5-) A (1-4) Q (0-) N (0-) O (0-) S (0-) P, AR (1-),
          BD (2-) D, RC (1-), RS (0-) E5 (0-) E6> (SO G6) / 258
  251-G5
 G39
        = Ak < BD (0-) D (0-) T > (SO) / 256
 H_{\frac{2}{2}} C_{\frac{6}{6}} R
        = Ak < BD (0-) D (0-) T> (SO) / OH / F / Cl / Br / I / H
G41
        = alkyl
G42
        = R / (SC NH2 / OH / CO2H / acyl / aryl / Ph (SO) /
          heteroaryl / CONH2 / alkoxycarbonyl / dialkylaminocarbonyl /
          F / Cl / Br / I / OH)
G43
       = R / (SC aryl / heteroaryl)
G44
       = OH / alkoxy
G45
       = Ph (SO)
G46
       = R / (SC Ak (SO) / NO2 / F / Cl / Br / I / NH2 (SO) /
          alkoxy (SO) / CO2H (SO) / aryl (SO) / Hy (SO) / CN /
          alkoxycarbonyl (SO) / CONH2 (SO) / alkylcarbonyl (SO))
G47
       = R / (SC NH2 (SO) / arylcarbonylamino /
         alkylcarbonylamino)
MPL:
         claim 1
NTE:
         and pharmaceutically acceptable salts
         substitution is restricted
NTE:
         additional substitution and ring formation also claimed
NTE:
         also incorporates later claims
L37 ANSWER 7 OF 25 MARPAT COPYRIGHT 2005 ACS on STN
     137:375233 MARPAT Full-text
AN
TΙ
     Metal substituted non centrosymmetrical phthalocyanine analogues, their
     preparation and use in photodynamic therapy and in vivo diagnostic
     Roncucci, Gabrio; Dei, Donata; De Filippis, Maria Paola; Fantetti, Lia;
IN
     Nistri, Daniele
PΑ
     L. Molteni & C. Dei Fratelli Alitti Societa' di Esercizio S.P.A., Italy
SO
     PCT Int. Appl., 36 pp.
     CODEN: PIXXD2
DT
     Patent
     English
LA
FAN.CNT 1
```

APPLICATION NO. DATE

PATENT NO.

KIND DATE

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ΡI
               WO 2002090361
                                                                   A1
                                                                                   20021114
                                                                                                                              WO 2002-EP3108 20020320
               WO 2002090361
                                                                  C1
                                                                                   20040521
                           W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
                                       CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
                                       GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
                                       LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
                                       PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
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               CA 2441386
                                                                  AA
                                                                              20021114
                                                                                                                             CA 2002-2441386 20020320
               EP 1381611
                                                                   A1
                                                                                  20040121
                                                                                                                             EP 2002-750855 20020320
                                 AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
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               JP 2004529171
                                                               T2 20040924
                                                                                                                           JP 2002-587440
                                                                                                                                                                               20020320
               ZA 2003008093
                                                                  Α
                                                                                 20040708
                                                                                                                          ZA 2003-8093
              US 2004156787
                                                               A1
                                                                                 20040812
                                                                                                                        US 2004-472882
                                                                                                                                                                               20040401
PRAI EP 2001-106411
                                                                20010321
              WO 2002-EP3108
                                                           20020320
     MSTR 1A
   942-G15-944
G1
                   = H / G7 / 58 / 60 / (SC 843 / pyridyl / 495 / 502 /
                          510 / 518 / 521 / 533 / 552 / 565 / 2-imidazolyl / 569 /
                         578 / 591 / 609 / 94 / 132 / 640 / 142 / 204 / 176 / 199 /
                         653 / 662 / NMe2 / 675 / 679 / 710 / 772)
                                                            H_{\mathcal{G}}G CH_2 G_{10}
                                                                      176
                                                                       P-66H4NH2
m_{\bar{5}} = 10^{-4} \text{Me} \text{ e}^{-1} \text{ m}_{\bar{5}} = 10^{-4} \text{ m}_{
```

Me Me
$$CH_2$$
 Me Me CH_2 Me Me

$$G5 = O / NH (SO) / S$$

 $G6 = NMe2 / 536 / 626 / 631$

Me
$$\begin{array}{c}
Me \\
+ \\
Me
\end{array}$$
Me
$$\begin{array}{c}
Me \\
+ \\
Me
\end{array}$$
Me
$$\begin{array}{c}
G_3 \{0\} - NH - CH_2 - CH_2 - NH_2
\end{array}$$
Me
$$\begin{array}{c}
Me \\
Me
\end{array}$$
Me
$$\begin{array}{c}
Me \\
Me
\end{array}$$
Me

G7 = Hy<EC (-2) Q (0-) N (0-) O (0-) S (0) OTHERQ> (SO) / 368 / 373 / 380 / 382 / 404 / 411 / 418 / (EX morpholino / piperidino / pyridyl / pyrimidinyl / piperazino / pyrrolidino / 422 / 427 / imidazolyl / NHPh / 432 / 444 / 456 / 481 / 493)

$$404$$

$$G21$$

$$411$$

$$G21$$

$$418$$

$$G21$$

$$422$$

$$427$$

$$432$$

$$432$$

$$432$$

$$432$$

G8 = Zn G9 = NMe2 / NEt2 / 644 / 649

G10 = O / CH2 G11 = 681 / pyridyl / 690 / 696 / 709 / 717 / 729 / 730 / 736 / 753 / 756 / 771 / 782

$$H_{\frac{2}{7}}CH_{2}-N-Me$$
 $H_{\frac{2}{7}}CH_{2}-CH_{2}-CH_{2}-CH_{2}-CH_{2}-NH_{2}$
 $P_{\frac{7}{3}}GH_{4}C(0).NH-CH_{2}-CH_{2}-NH_{2}$

G12 = 351 / 352 / 357

$$3^{+}_{51} \stackrel{?}{\longrightarrow} G8$$
 G1 3 $\frac{+}{3} \stackrel{?}{\longrightarrow} 0^{-}$ G1 4 G1 4 -0^{-} $3^{+}_{51} \stackrel{?}{\longrightarrow} 0^{-}$ G1 4

G13 = A1

G14 = H / alkyl < (1-15) >

G15 = 26-942 25-944 / 971-942 968-944 / 1017-942 1018-944 / 1083-942 1080-944

G16 = H / R

G17 = 863 / SH / OH / NH2 / 858 / 788 / 876 /

R<TX "imidate or biotine"> / 873 / Ph (SR OH) / OPh (SO) / (SC 898 / 899 / 910 / 929 / 939 / 940)

$$_{9}^{C}$$
 $_{9}^{C}$ $_{1}^{G}$ $_{1}^{G}$ $_{1}^{G}$ $_{2}^{G}$ $_{1}^{G}$ $_{2}^{G}$ $_{3}^{G}$ $_{1}^{G}$ $_{1}^{G}$ $_{2}^{G}$ $_{3}^{G}$ $_{1}^{G}$ $_{2}^{G}$ $_{3}^{G}$ $_{4}^{G}$ $_{1}^{G}$ $_{4}^{G}$ $_{4}^{G}$

G19 =
$$H / alkyl < (1-15) > / Ph$$

$$G20 = alkylene < (1-10) > (SO (-2) G22)$$

$$G21 = 385 / 390 / 397$$

$$385$$
 G_{19} H_{390} $N_{G_{19}}$ G_{19} G_{19} G_{19} G_{19} G_{19} G_{19}

G22 =
$$R / (-2)$$
 G21
G23 = $R / (SC 889)$

$$G27 = NMe2 / 853$$

MPL: claim 1

NTE: additional ring formation also claimed

NTE: substitution is restricted

NTE: and pharmaceutically acceptable salts

RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD

```
ALL CITATIONS AVAILABLE IN THE RE FORMAT
L37 ANSWER 8 OF 25 MARPAT COPYRIGHT 2005 ACS on STN
    137:140527 MARPAT Full-text
    Preparation of alkylcarbamic acid esters as acetylcholinesterase inhibitor
    and serotonin reuptake inhibitor
    Koyama, Kazuo; Marumoto, Shinji; Toda, Narihiro; Kogen, Hiroshi; Suzuki,
IN
    Keiko
    Sankyo Company, Limited, Japan
PA
so
    PCT Int. Appl., 300 pp.
    CODEN: PIXXD2
DT
    Patent
LA
    Japanese
FAN.CNT 1
    PATENT NO.
                  KIND DATE
                                      APPLICATION NO. DATE
    -----
                                       ______
    WO 2002059074
                                      WO 2002-JP400 20020122
                   A1 20020801
        W: AU, BR, CA, CN, CO, CZ, HU, ID, IL, IN, KR, MX, NO, NZ, PH, PL,
           RU, SG, SK, US, VN, ZA
        RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
           PT, SE, TR
                    AA 20020801
                                       CA 2002-2435883 20020122
    CA 2435883
    EP 1362844
                   A1 20031119
                                      EP 2002-716323 20020122
        R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
           IE, FI, CY, TR
                   A2 20030624
    JP 2003176256
                                       JP 2002-15136
                                                       20020124
                                      US 2003-629108
    US 2004067981
                    A1
                         20040408
                                                      20030728
PRAI JP 2001-18386
                   20010126
    JP 2001-305182
                   20011001
    WO 2002-JP400
                  20020122
 MSTR 1
    G15
        = alkyl<(1-6)> / NH2 / alkylamino<(1-6)> /
```

∵•

$$G2 = 13-3 14-6 / 16 / (EX 63-3 70-6)$$

(SC 19) / (EX morpholino)

G3 =
$$aryl<(-14)>$$
 (SO (1-5) G4) / heteroaryl (SO (1-3) G4) / (SC Ph (SO (1-3) G18) / pyridyl (SO (-1) G4) / 35 / 43) / (EX 49 / naphthyl / 57)

```
G19
       = F / Cl / Br / I / alkyl < (1-6) > (SO (1-) G5) /
G4
         alkoxy<(1-6)> / alkylthio<(1-6)> / CHO /
         alkylcarbonyl<(1-6)> / alkoxycarbonyl<(1-6)> / NH2 / NHCHO /
         alkylcarbonylamino<(1-6)> / OH / SH / CN / NO2 / CO2H
       = F / Cl / Br / I
       = alkylene<(1-6)> / 9-4 10-7 / (SC CH2 / CH2CH2)
G6
 67-168
       = alkylene<(1-6)> / (SC CH2 / CH2CH2)
       = 0 / S / NH / 11
 11-G9
       = CHO / alkylcarbonyl<(1-6)>
G9
G10
       = phenylene (SO (-1) G11)
       = alkyl < (1-6) > / alkenyl < (2-6) > / (SC Me)
G11
G12
       = NH2 / 22 / 24
 ₽Ŋ----G17
       = Hy<EC (1) N (8-10) C, AN (1) N, BD (60) D, RC (2-),
G13
         RS (1-) E6>
       = H / alkyl < (1-6) > / (SC Me / Et)
G14
       = 0 / s
G15
       = Me / Et
G16
G17
       = alkyl<(1-6)> / (SC Me / Et)
       = F / Cl / Br / I / alkyl<(1-6)> (SO (1-) G5) /
G18
         alkoxy<(1-6)> / alkylthio<(1-6)> / CHO /
         alkylcarbonyl<(1-6)> / alkoxycarbonyl<(1-6)> / NH2 / NHCHO /
         alkylcarbonylamino<(1-6)> / OH / SH / CN / NO2 / CO2H / Me /
         CF3 / OMe / SMe / COMe
G19
       = alkylene<(1-3)>
G20
       = G22 / 72-65 74-69
 \mu\varsigma = CH - \gamma \zeta H_2
G21
       = H / Me
G22
       = (1-3) CH2
MPL:
         claim 1
NTE:
         additional ring formation also claimed
         or pharmacologically acceptable salts or esters
NTE:
RE.CNT 3
              THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
              ALL CITATIONS AVAILABLE IN THE RE FORMAT
L37 ANSWER 9 OF 25 MARPAT COPYRIGHT 2005 ACS on STN
     136:232317 MARPAT Full-text
ΑN
     Preparation of heterocyclylbenzenes as herbicides and defoliants.
ΤI
```

```
Gupta, Sandeep; Wu, Shao-Yong; Tsukamoto, Masamitsu; Pulman, David A.;
     Ying, Bai-Ping
PA
     ISK Americas Incorporated, USA
SO
     U.S., 74 pp., Cont.-in-part of U.S. Ser. No. 958,313.
     CODEN: USXXAM
DΨ
     Patent
     English
LA
FAN.CNT 2
     PATENT NO.
                    KIND DATE
                                         APPLICATION NO. DATE
     US 6355799
                     B1 20020312
                                         US 2000-530373 20000427
     WO 9921837
                     A1 19990506
                                         WO 1998-US17197 19980821
        W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE,
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            KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX,
            NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT,
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            FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI,
             CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                         US 2001-930149 20010816
     US 2002133007
                     A1
                           20020919
     US 6545161
                            20030408
                      В2
PRAI US 1997-958313
                     19971027
     WO 1998-US17197 19980821
     US 2000-530373
                     20000427
  MSTR 1
G1
      = H / F / Cl / Br / I / NO2 / NH2 / 8 / 10 / CONH2 /
        CSNH2 / CN / alkylcarbonyl < (1-8) > / alkoxycarbonyl < (1-8) > /
        alkylaminosulfonyl < (1-8) > / alkyl < (1-8) > (SO (1-) G3) / \\
        alkoxy<(1-8)>(SO(1-)G3)/alkoxy<(1-8)>
         (SR alkoxycarbonyl<(1-8)> (SO)) / OCH2Ph (SO) /
        aryloxy<(6-10)> (SO) / heteroaryloxy<EC (1-4) Q (0-) N (0-)
        O(0-) S(0) OTHERQ>(SO)
 = alkyl<(1-8)>(SO) / alkenyl<(2-8)>(SO) /
G2
        alkynyl<(2-8)> (SO) / Cb<EC (3-8) C, AR (0)> (SO) /
        aryl<(6-10)> (SO) / heteroaryl<EC (1-4) Q (0-) N (0-) O (0-)
        S (0) OTHERQ> (SO) / 13 / alkylsulfonyl<(1-8)> (SO) /
        CH2Ph (SO) / alkylcarbonyl<(1-8)> (SO) /
        alkenylcarbonyl<(2-8)>(SO) / alkynylcarbonyl<(2-8)>(SO) /
        arylcarbonyl<(6-10)> (SO) / heteroarylcarbonyl<EC (1-4)
        Q (0-) N (0-) O (0-) S (0) OTHERQ> (SO) /
        alkoxycarbonyl<(1-8)> (SO) / aryloxycarbonyl<(6-10)> (SO) /
        heteroaryloxycarbonyl<EC (1-4) Q (0-) N (0-) O (0-) S (0)
        OTHERQ> (SO)
```

```
= F / Cl / Br / I / R
G3
G4
       = F / Cl / Br / I
G5
       = alkyl<(1-8)>(SO) / Cb<EC (3-8) C, AR (0)>(SO) /
         aryl<(6-10)> (SO) / heteroaryl<EC (1-4) Q (0-) N (0-) O (0-)
         S (0) OTHERQ> (SO)
       = H / F / Cl / Br / I / NO2
G6
       = H / OH / SH / NH2 / 17 / Me /
G7
         Ak < EC (1-) C, BD (0-) D (0-) T > (SO (1-3) G9) / F / Cl / Br /
         I / NO2 / CN / (SC 303 / OMe)
 198-G2 383-G27
       = 0 / s / NH / 19
G8
```

1 N ----- G2

G9 = R / Cb<EC (3-8) C, AR (0)> (SO) /
aryl<(6-10)> (SO) / heteroaryl<EC (1-4) Q (0-) N (0-) O (0-)
S (0) OTHERQ> (SO) / 21 / alkylsulfonyl<(1-8)> (SO) /
CH2Ph (SO) / alkylcarbonyl<(1-8)> (SO) /
alkenylcarbonyl<(2-8)> (SO) / alkynylcarbonyl<(2-8)> (SO) /
arylcarbonyl<(6-10)> (SO) / heteroarylcarbonyl<EC (1-4)
Q (0-) N (0-) O (0-) S (0) OTHERQ> (SO) /

Q (0-) N (0-) O (0-) S (0) OTHERQ> (SO) / alkoxycarbonyl<(1-8)> (SO) / aryloxycarbonyl<(6-10)> (SO) / heteroaryloxycarbonyl<EC (1-4) Q (0-) N (0-) O (0-) S (0) OTHERQ> (SO)

29----G5

G10 = 25 / 202 / 212 / (EX Hy (SO) / 37 / 46 / 55 / 62 / 71 / 82 / 93 / 104 / 122 / 133 / 144 / 155 / 166 / 169 / 179 / 190 / 272 / 283 / 294 / phthalimido / 222 / 231)

= H / alkyl < (1-8) > (SO (1-) G4) / alkenyl < (2-8) > /G11 alkynyl<(2-8)> / NH2 / alkyl<(1-8)> (SR alkoxy<(1-8)>) /COMe / alkoxycarbonylamino<(1-8)> / alkylcarbonylamino<(1-8)> / alkoxycarbonyl<(1-8)> / (SC Me) G12 = alkyl < (1-8) > (SO (1-) G4) / (SC CF3)= H / F / Cl / Br / I / NO2 / NH2 / G13 alkylamino<(1-8)> (SO (1-) G4) / CN / CONH2 = 0 / S / NH G14 = N / CH G15 = NH2 / OH / SH / CHO / CO2H / CN / G16 alkylcarbonyl<(1-8)> / arylcarbonyl<(6-10)> / N3 / 242 / Hy < EC (4-8) A (1-) Q (1-) N, AN (1) N > / 258 /Ak<EC (1-) C, BD (0-) D (0-) T> (SO (1-) G25) / NO2 / (SC 305)

$$2^{\frac{G}{4}}2^{7}$$
-G18 G^{24} G^{23} $H_{\frac{3}{5}}G_{\frac{5}{5}}$ -G29

$$G17 = NH / 244 / O / S$$

```
= alkyl<(1-8)>(SO) / alkenyl<(2-8)>(SO) /
G18
         alkynyl<(2-8)>(SO) / NH2(SO) /
         Cb<EC (3-8) C, AR (0)> (SO) / Hy<EC (3-8) A (1-4) Q (0-)
         N (0-) O (0-) S (0) OTHERQ, AR (0) > (SO) /
         alkylsulfonyl<(1-8)> (SO) / arylsulfonyl<(6-10)> (SO) /
         CH2Ph (SO) / \text{ aryl} < (6-10) > (SO) /
         heteroary1<EC (1-4) Q (0-) N (0-) O (0-) S (0) OTHERQ> (SO) /
         alkylcarbonyl<(1-8)>(SO) / alkenylcarbonyl<(2-8)>(SO) /
         alkynylcarbonyl<(2-8)> (SO) / 246 / 250 / 255
 2960).G19
               _G20 2550)-C(0)-G22
G19
       = Cb < EC (3-8) C, AR (0) > (SO) / aryl < (6-10) > (SO) /
         heteroaryl<EC (1-4) Q (0-) N (0-) O (0-) S (0) OTHERQ> (SO) /
         248 / alkylthio<(1-8)>(SO) / arylthio<(6-10)>(SO) /
         NH2 (SO) / 253
 29<del>8</del> G5
          = aryl < (6-10) > (SO)
G20
       = alkyl < (1-8) > (SO) / aryl < (6-10) > (SO) /
G21
         heteroaryl<EC (1-4) Q (0-) N (0-) O (0-) S (0) OTHERQ> (SO)
G22
       = alkoxy<(1-8)> (SO) / aryl<(6-10)> (SO)
       = alkyl<(1-8)> (SO (1-) G4) / dialkylamino<(1-8)> /
G23
         aryl < (6-10) > (SO) / heteroaryl < EC (1-4) Q (0-) N (0-) O (0-)
         S (0) OTHERQ> (SO)
       = H / F / Cl / Br / I / alkyl < (1-8) > (SO (1-) G4) /
G24
         dialkylamino<(1-8)> / aryl<(6-10)> (SO) /
         heteroaryl<EC (1-4) Q (0-) N (0-) O (0-) S (0) OTHERQ> (SO)
       = CO2H / R / NH2 (SO) / Cb < EC (3-8) C, AR (0) > (SO) /
G25
         Hy<EC (3-8) A (1-4) Q (0-) N (0-) O (0-) S (0) OTHERQ,
         AR (0) > (SO) / alkylsulfonyl<(1-8) > (SO) /
         arylsulfonyl<(6-10)> (SO) / CH2Ph (SO) / aryl<(6-10)> (SO) /
         heteroaryl<EC (1-4) Q (0-) N (0-) O (0-) S (0) OTHERQ> (SO) /
         alkylcarbonyl<(1-8)>(SO) / alkenylcarbonyl<(2-8)>(SO) /
         alkynylcarbonyl<(2-8)> (SO) / 262 / 264 / 267
 2620).G19
               _G20 <sub>2</sub>G60)⋅C(0)⋅G22
G26
       = O / S / (EX NH)
       = alkyl < (1-8) > (SO (1-) G28) /
G27
         alkenyl<(2-8)> (SO (1-) G28) / alkynyl<(2-8)> (SO (1-) G28)
       = F / Cl / Br / I / CN / NO2 / NH2 / CO2H
G28
       = CO2H / alkyl < (1-8) > (SO) / alkenyl < (2-8) > (SO) /
G29
         alkyny1<(2-8)>(SO) / NH2(SO) /
         Cb<EC (3-8) C, AR (0)> (SO) / Hy<EC (3-8) A (1-4) Q (0-)
         N (0-) O (0-) S (0) OTHERQ, AR (0) > (SO) /
         alkylsulfonyl<(1-8)>(SO) / arylsulfonyl<(6-10)>(SO) /
         CH2Ph (SO) / \text{ aryl} < (6-10) > (SO) /
         heteroaryl<EC (1-4) Q (0-) N (0-) O (0-) S (0) OTHERQ> (SO) /
         alkylcarbonyl<(1-8)>(SO) / alkenylcarbonyl<(2-8)>(SO) /
         alkynylcarbonyl<(2-8)>(SO) / 307 / 309 / 312
```

. `

```
or salts
DER:
MPL:
        claim 1
NTE:
        additional ring formation also claimed
NTE:
        substitution is restricted
NTE:
        also incorporates claim 9 and broader disclosure
             THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE.CNT 37
             ALL CITATIONS AVAILABLE IN THE RE FORMAT
L37
    ANSWER 10 OF 25 MARPAT COPYRIGHT 2005 ACS on STN
    135:132442 MARPAT Full-text
ΤI
    Compounds exhibiting thrombopoietin receptor agonism
IN
    Takemoto, Hiroshi; Shiota, Takeshi; Takayama, Masami
PΑ
    Shionogi & Co., Ltd., Japan
    PCT Int. Appl., 352 pp.
SO
    CODEN: PIXXD2
DΨ
    Patent
LA
    Japanese
FAN.CNT 1
                                        APPLICATION NO. DATE
    PATENT NO.
                   KIND DATE
    -----
                    ----
                                         -----
                                        WO 2001-JP411 20010123
    WO 2001053267
                    A1 20010726
PΙ
        W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
            CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR,
            HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU,
            LV, MZ, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD,
            SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU,
            ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
        RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
            DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
            BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                    AA 20010726 CA 2001-2397018 20010123
    CA 2397018
                                        AU 2001-27089
    AÚ 2001027089
                     Α5
                          20010731
                                                         20010123
    AU 777777
                     B2
                          20041028
                                                         20010123
    EP 1253142
                     A1
                         20021030
                                        EP 2001-901511
        R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
                                        US 2002-169362
                                                          20020702
    US 2003195231
                    A1 20031016
PRAI JP 2000-13770
                     20000124
    JP 2000-30593
                     20000208
    WO 2001-JP411
                    20010123
 MSTR 1A
 G1-G3-G15-G22
      = aryl (SO) / heteroaryl<EC (0-) N (0-) O (0-) S>
G1
        (SO) / (SC pyridyl (SO (-2) G17) / 256 /
```

2-thienyl (SO (-2) G17) / 281 / 286 / 291 / 500 / 507 /

536) / (EX 640)

G3 = 5-1 8-3 / 16-1 14-3 / 435-1 431-3 / 22-1 20-3 / 440-1 437-3 / 24-1 26-3 / 442-1 443-3 / 28-1 31-3 / 461-1 474-3 / 465-1 475-3 / 476-1 468-3 / 477-1 470-3 / 455-1 456-3 / 459-1 458-3 / 38-1 39-3 / 452 / 41-1 43-3 / 47-1 49-3 / 54-1 57-3 / 60-1 65-3 / 66-1 70-3 / 74-1 77-3 / (SC 487-1 488-3)

$${}_{4}\ddot{g}\ddot{f}\underline{\qquad}{}_{G}^{G}\underline{\qquad}{}_{A}\ddot{g}\dot{f}^{O}) \\ {}_{4}\ddot{q}\ddot{g}\underline{\qquad}{}_{G}\underline{\qquad}{}$$

```
= H / loweralkyl (SO)
G4
       = NULL / alkylene<(1-)> (SO) / O / S / 9-6 10-3 /
         CH=CH (SO)
 G6-167
       = alkylene<EC (1-2) C, DC (0) M3>
       = 0 / s
G7
       = alkylene<EC (1-5) C, DC (0) M3>
G8
       = 29-28 30-31 / 36-28 35-31
G10
       = 0 / S
G11
      = SH / loweralkylthio (SO)
G12
G14
       = C(S) / CH2 / CH2CH2
G15
       = phenylene (SO (-2) G49) /
         heteroarylene<EC (0-) N (0-) O (0-) S, RC (1)> (SO) /
         Hy < EC (0-) N (0-) O (0-) S, AR (0), RC (1),
         RS (0-) E5 (0-) E6 (0-) E7 (0) OTHER> (SO) /
         cycloalkylene<RC (1) > (SO) / (SC 620-2 617-541 /
         626-2 623-541 / 628-2 630-541 ) / (EX 673-2 670-541 /
         681-2 678-541 )
       = H / loweralkyl (SO) / CO2H / loweralkoxycarbonyl /
G16
         F / Cl / Br / I / CONH2 (SO) / heteroaryl<EC (0-) N (0-)
         0 (0-) S> (SO) / aryl (SO)
       = loweralkyl (SO) / CO2H / loweralkoxycarbonyl / F /
G17
         Cl / Br / I / CONH2 (SO) / heteroaryl<EC (0-) N (0-) O (0-)
         S> (SO) / aryl (SO)
G18
       = H / Ph
G19
       = s / 485
 485-G20
       = H / loweralkyl
G20
       = 542 / 601 / 603 / 605 / 607 / aryl (SO) /
G22
         heteroary1<EC (0-) N (0-) O (0-) S> (SO) / 612
```

.

```
5923—G27 6810).G39 6830).G42 6830).G43 G40 028—N—G40
```

6 G 4 6=N----O---G 4 1 G23 = Ak<(2-)> (SO (-2) G24) / ethynylene= F / Cl / Br / I / loweralkoxy (SO) / G24 loweralkylthio (SO) / aryl (SO) / heteroaryl<EC (0-) N (0-) O (0-) S> (SO) / cycloalkyl (SO) / Hy < EC (0-) N (0-) O (0-) S, AR (0) > / NH2 (SO)G25 = H / loweralkyl (SO) / CO2H / loweralkoxycarbonyl / F / Cl / Br / I / CONH2 (SO) = aryl (SO) / heteroaryl<EC (0-) N (0-) O (0-) S> G26 (SO) / R = 652 / 654 / 656 / 658 / aryl (SO) / G27 heteroaryl<EC (0-) N (0-) O (0-) S> (SO) / (EX 663)65(0)-G39 65(0)-G42 65(0)-G43 G40 G40 G63N G40 H = H / alkyl (SO) / cycloalkyl / alkoxy (SO) / G28 alkylthio / F / Cl / Br / I / Ph (SO) / heteroaryl<EC (0-) N (0-) O (0-) S> (SO) / Hy < EC (0-) N (0-) O (0-) S, AR (0) > (SO)= H / loweralkyl (SO) / CO2H / loweralkoxycarbonyl / G29 F / Cl / Br / I / CONH2 (SO) / CF3 = H / alkyl (SO) / cycloalkyl / alkoxy (SO) / G30 alkylthio / F / Cl / Br / I / Ph (SO) / heteroaryl<EC (0-) N (0-) O (0-) S> (SO) / Hy < EC (0-) N (0-) O (0-) S, AR (0) > (SO)= H / alkyl (SO) / cycloalkyl / alkoxy (SO) / G31 alkylthio / F / Cl / Br / I / Ph (SO) / heteroaryl<EC (0-) N (0-) O (0-) S> (SO) /Hy < EC (0-) N (0-) O (0-) S, AR (0) > (SO)G34 = 0 / s= (1) Ph (SO (1-) G37) / H / loweralkyl <math>(SO) / CO2H /G36 loweralkoxycarbonyl / F / Cl / Br / I / CONH2 (SO) = alkyl (SO) / cycloalkyl / alkoxy (SO) / alkylthio / G37 F / Cl / Br / I / Ph (SO) / heteroaryl<EC (0-) N (0-) O (0-) S> (SO) / Hy < EC (0-) N (0-) O (0-) S, AR (0)> (SO) G39 = 632 / OH / 635 G_{40} G_{5} G_{41} = H / F / Cl / Br / I / loweralkyl (SO) /G40 loweralkoxy (SO) / loweralkylthio (SO) / loweralkenyl (SO) / loweralkynyl (SO) / aryl (SO) / heteroaryl<EC (0-) N (0-) O (0-) S> (SO) / cycloalkyl (SO) / alkyl (SR G26) / Hy<EC (0-) N (0-) O (0-) S, AR (0)> / NH2 (SO)

= loweralkyl (SO) / loweralkenyl (SO) /

loweralkynyl (SO) / aryl (SO) /

G41

```
heteroaryl<EC (0-) N (0-) O (0-) S> (SO) / cycloalkyl (SO) /
         alkyl (SR G26) / Hy<EC (0-) N (0-) O (0-) S, AR (0)> (SO)
G42
       = loweralkyl (SO) / loweralkenyl (SO) /
         loweralkynyl (SO) / alkyl (SR G26)
       = H / aryl (SO) / heteroaryl < EC (0-) N (0-) O (0-) S >
G43
         (SO) / cycloalkyl (SO) / Hy<EC (0-) N (0-) O (0-) S, AR (0)>
         (SO) / (EX morpholino)
       = Ak < (3-) > (SO (-3) G24)
G46
       = 2-furyl / 649
G47
       = 0 / CH2
G48
       = R / (SC loweralkyl (SO (1-) G50) / F / Cl / Br / I /
G49
         loweralkoxy (SO (1-) G50) / OH)
G50
       = F / Cl / Br / I
G29+G30= alkylene<(1-3)> / 521-505 520-510 / 523-505 522-510
 H_{\frac{5}{2}}C_{0} = 5C_{\frac{3}{4}}^{\frac{4}{5}} 5C_{\frac{3}{4}}C_{\frac{3}{5}}C_{\frac{3}{4}}^{\frac{4}{5}}
MPL:
         claim 1
NTE:
         or prodrugs, pharmaceutically acceptable salts or solvates
              THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE.CNT 14
              ALL CITATIONS AVAILABLE IN THE RE FORMAT
L37 ANSWER 11 OF 25 MARPAT COPYRIGHT 2005 ACS on STN
     134:353257 MARPAT Full-text
     4-Phenyltetrahydroisoquinolines and use thereof to block reuptake of
     norepinephrine, dopamine and serotonin
IN
     Beck, James P.; Smith, Mark A.
     Du Pont Pharmaceuticals Company, USA
PA
     PCT Int. Appl., 79 pp.
     CODEN: PIXXD2
DT
     Patent
     English
FAN.CNT 1
     PATENT NO.
                                           APPLICATION NO. DATE
                     KIND DATE
                                            _____
     ______
                                           WO 2000-US30328 20001103
                     A1 20010510
PΙ
     WO 2001032624
         W: AU, BR, CA, CN, CZ, EE, HU, IL, IN, JP, KR, LT, LV, MX, NO, NZ,
             PL, RO, SG, SI, SK, TR, UA, VN, ZA, AM, AZ, BY, KG, KZ, MD, RU,
             TJ, TM
         RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
             PT, SE, TR
                                            CA 2000-2389300 20001103
     CA 2389300
                       AA
                            20010510
                                                              20001103
                                            BR 2000-15307
     BR 2000015307
                       Α
                            20020709
                                            EP 2000-976884
                                                              20001103
     EP 1246805
                       Α1
                            20021009
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, CY, TR
                                           JP 2001-534776
                                                              20001103
     JP 2004501860
                      Т2
                            20040122
                                           NZ 2000-519146
                                                              20001103
     NZ 519146
                       Α
                             20040227
PRAI US 1999-163270P 19991103
     WO 2000-US30328 20001103
```

= alkyl < (1-6) > (SO (1-3) G2) / alkenyl < (2-6) > (SO) /G1 alkynyl<(2-6)>(SO) / cycloalkyl<(3-6)>(SO) /alkyl < (1-6) > (SR G3) / (SC Me / CF3)= alkyl<(1-3)> / F / Cl / Br / I / Ph (SO) / CN / OH / G2

25 / 28 / piperidino / pyrrolidino / piperazino / 132 / morpholino / thiomorpholino

= (1-) cycloalkyl<(3-7)> (SO) / R G3

= H / alkyl < (1-6) > / alkenyl < (2-6) > / alkynyl < (2-6) > /G4 cycloalkyl<(3-6)>/alkyl<(1-6)>(SR cycloalkyl<(3-7)>)/alkyl < (1-6) > (SR (1-) G22) / (SC Me)

= H / F / Cl / Br / I / OH / 38 / SH / 142 / 145 / G5 40 / 42 / CN / 46 / 50 / alkyl<(1-6)> (SO (1-3) G2) / alkenyl<(2-6)>(SO) / alkynyl<(2-6)>(SO) /cycloalkyl<(3-6)>(SO) / alkyl<(1-6)>(SR G3) /OPh (SO (1-3) G6) / 35 / (SC Me / Et / Pr-n / Pr-i / OMe / CF3 / 189 / 192)

= F / Cl / Br / I / CN / alkyl<(1-4)> /G6 alkyl<(1-4)> (SR (1-) G22) / alkoxy<(1-4)>

G7 = Ph (SO)

= S / S(0) / SO2G8

= H / F / Cl / Br / I / OH / 52 / SH / 147 / 150 / G9 54 / 56 / CN / 60 / 64 / 66 / piperidino / pyrrolidino / piperazino / 178 / morpholino / thiomorpholino / alkyl < (1-6) > (SO (1-3) G2) / alkenyl < (2-6) > (SO) /alkynyl<(2-6)>(SO) / cycloalkyl<(3-6)>(SO) /Pr-n / Pr-i / CF3 / 195 / CH2OH)

G10 = H / F / Cl / Br / I / OH / 72 / SH / 152 / 155 /
74 / CN / 76 / 78 / piperidino / pyrrolidino / piperazino /
185 / morpholino / thiomorpholino / 83 / 86 / 89 /
alkyl<(1-6)> (SO) / alkenyl<(2-6)> (SO) /
alkynyl<(2-6)> (SO) / cycloalkyl<(3-6)> (SO) /
alkyl<(1-6)> (SR cycloalkyl<(3-7)> (SO)) / F / Cl / Me /
(SC OMe / CF3)

$$72$$
—G14 74 8—G16 76 (0)G15 6 13 6 13 6 13 6 13 6 15 6 15 6 16 6 17 6 17 6 18 6 18 6 19

G11 = 11 / 93 / 102

$$G10$$
 $G10$
 $G10$
 $G10$
 $G10$
 $G15$
 $G21$
 $G21$
 $G21$
 $G21$

195-G14

H257 G7 1560)-G19

G14 =
$$alkyl<(1-4)>$$
 / $alkyl<(1-4)>$ (SR (1-) G22) / $alkyl<(1-4)>$ (SR $alkoxy<(1-4)>$) / $cycloalkyl<(3-6)>$ / $alkyl<(1-6)>$ (SR $cycloalkyl<(3-7)>$) / 138 / Ph (SO) / 119

H2f9-G7 1960)-G19

G15 = H / NH2 / alkyl<
$$(1-4)$$
> / alkyl< $(1-4)$ > (SR (1-) G22) / alkyl< $(1-4)$ > (SR alkoxy< $(1-4)$ >

```
) / cycloalkyl<(3-6)> / alkyl<(1-6)> (SR cycloalkyl<(3-7)>) /
        159 / Ph (SO) / 163
 1860)-G19 H263-G7
G16
      = NH2 / alkyl < (1-4) > / alkyl < (1-4) > (SR (1-) G22) /
        alkyl<(1-4)>(SR alkoxy<(1-4)>) / cycloalkyl<(3-6)> /
        alkyl<(1-6)> (SR cycloalkyl<(3-7)>) / 161 / Ph (SO) / 165
 16(0)-G19 H2C-G7
G17
      = OH / 157
 18<del>7--</del>G16
      = 43 / piperidino / pyrrolidino / piperazino / 170 /
G18
        morpholino / thiomorpholino
G19
      = alkyl < (1-4) > (SO (1-) G22) / Ph
G20
      = NHMe / NMe2
      = H / R
G21
      = F / Cl / Br / I
G22
MPL:
       claim 1
       substitution is restricted
NTE:
        or oxides, pharmaceutically acceptable salts, solvates, or prodrugs
NTE:
STE:
       7 - R or S
             THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE.CNT 11
             ALL CITATIONS AVAILABLE IN THE RE FORMAT
L37 ANSWER 12 OF 25 MARPAT COPYRIGHT 2005 ACS on STN
    134:296229 MARPAT Full-text
TΙ
    Polymerizable mesogenic tolans
IN
    Farrand, Louise Diane
    Merck Patent Gmbh, Germany
    Brit. UK Pat. Appl., 34 pp.
    CODEN: BAXXDU
DT
    Patent
    English
LA
FAN.CNT 1
                                         APPLICATION NO. DATE
     PATENT NO.
                 KIND DATE
                     ----
                                         _____
     -----
                                        GB 2000-16160
                                                          20000630
    GB 2351734
                    A1 20010110
PΙ
                    B2 20040901
     GB 2351734
    US 6514578
                     B1 20030204
                                     US 2000-598449 20000622
PRAI EP 1999-112455 19990630
```

MSTR 1B

•

$$G15$$
 $G15$
 $G15$

G1 = 19 / 24 / 27 / 29 / 34 / 39

 $H_2C = CH - \frac{1}{3} - \frac{$

```
G2 = H / Me / C1
```

G3 = phenylene

G4 = phenylene

G5 = O / S / C(O) / 40-38 41-1139 / 42-38 43-1139 / 44-38 45-1139 / 46-38 47-1139 / CH2CH2 / CH=CH / ethynylene / 48-38 51-1139 / 55-38 52-1139

$$46(0)_{4}66 \qquad 466-46(0) \qquad H_{4}2-467 \qquad 467-46H2 \qquad 49-C(0)-CH=5H$$

$$G6 = O / NH$$

G7 = 0 / S

G8 = R<TX "spacer group", EC (1-25) C> /

(SC alkylene<(1-12)>)
G9 = 59 / 64 / 67 / 69 / 73

$H_2C = CH - 7G^{11}$

G13 =
$$F / C1 / CN / OH / NO2 /$$

 $alky1<(1-7)> (SO (1-) G14) / alkoxy<(1-7)> (SO (1-) G14) /$
 $alky1carbony1<(1-7)> (SO (1-) G14) / CHO$

G14 = F / C1

```
G16 = 621-15 226-81 / 371-15 372-81
```

 $691^{4} + 692^{5} + 291^{7}$ $391^{0} + 392^{1}$

•

G23 = 609-529 610-372 / 611-529 612-372 / 613-529 616-372 / 617-529 620-372 / CH2CH2 / CH=CH / ethynylene

$$6998590$$
 $697-6928$ $693-C(0)-CH-698$ $697-C(0)-CH-698$

•

G27 = 859-779 860-622 / 861-779 862-622 / 863-779 866-622 / 867-779 870-622 / CH2CH2 / CH=CH / ethynylene

867-C(0)-CH-864 867-C(0)-CH-864 867-C(0)-CH-864

G28 = H / CN / X / Ak<EC (1-) C, BD (0) D (0-) T> (SO (1-) G29) / 873 / 875 / 879 / 882 / 883 / 886 / 889 / 893 / 900 / 905 / 908 / 910 / 914 / 919

8630-G31 8630-G31 8632-C(0)-G31 8633-G34-G35

G2—CH—CH—
$$g_{5}$$

G2—CH—G37— g_{1} 0 H2C—CH— g_{1} 38

G409G8-9G39

= X / CNG29 G30 = 0 / S / NH / NMe / OCO2G31 = alkyl<(-25)>(SO)G32 = 0 / s= alkylene<(-23)>(SO)G33 = O / S / NH / NMe / OCO2G34 = alkyl<(-23)>(SO)G35 G37 = phenylene G38 = phenylene = 0 / S / C(0) / 920-86 921-918 / 922-86 923-918 /G39 924-86 925-918 / 926-86 927-918 / CH2CH2 / CH=CH / ethynylene / 928-86 931-918 / 935-86 932-918

уç_СН—С(О)-92

= 939 / 944 / 947 / 949 / 953 G40

_С(О)дд₉ G2—СН—СН—9Q4 G2—947 H2С—СН—G41—9Q9

H2C==CH-9642

G41 = phenylene G42 = phenylene

claim 1 MPL:

substitution is restricted NTE:

additional interruptions of ak in G28 also claimed NTE:

L37 ANSWER 13 OF 25 MARPAT COPYRIGHT 2005 ACS on STN

130:338118 MARPAT Full-text

Preparation of heterocyclylbenzenes as herbicides and defoliants.

Gupta, Sandeep; Tsukamoto, Masamitsu; Pulman, David A.; Ying, Bai-ping; Wu, Shao-yong

ISK Americas Incorporated, USA

PCT Int. Appl., 139 pp.

CODEN: PIXXD2

DT Patent

English LA

FAN.	-	2																
	PAT	CENT :	NO.		KII	ND									DATE			
PI	wo	9921	 837		Α.	 L	1999					 98-U			1998	0821		
		W:	AL,	AM,	ΑT,	AU,	ΑZ,	BA,	BB,	BG,	BŔ,	BY,	CA,	CH,	CN,	CU,	CZ,	DE,
			DK,	EE,	ES,	FI,	GB,	GE,	GH,	GM,	HR,	HU,	ID,	IL,	IS,	JP,	KE,	KG,
			KP,	KR,	ΚZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MD,	MG,	MK,	MN,	ΜW,	MX,
															ТJ,			
			UA,	ŪG,	US,	UZ,	VN,	YU,	ZW,	AM,	ΑZ,	BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM
		RW:													CY,			
			FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,
							ML,											
		2307																
		9895								A)	U 19	98-9	5650		1998	0821		
		7492																
	ΕP	1030	843		A.	L	2000	0830		E	P 19	98-9	4930	2	1998	0821		
		R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙT,	LI,	LU,	NL,	SE,	MC,	PT,
			IE,															
	JР	2001	52102	27	T	2	2001	1106										
	BR	9814	104		Α		2001								1998	-		
	ZA	9809	639		Α										1998			
	TW	5332	00		В		2003	0521		T	W 19	98-8	7117	635	1998	1023		
		2204					2002	0630		E	G 19	98-1	309		1998	1027		
	US	6355	799		В:	L	2002	0312		U	s 20	00-5	3037	3	2000	0427		

```
US 2002133007 A1 20020919 US 2001-930149 20010816
US 6545161 B2 20030408

PRAI US 1997-958313 19971027
WO 1998-US17197 19980821
US 2000-530373 20000427

MSTR 1

G1  G6
```

40

G1 = H / F / Cl / Br / I / NO2 / NH2 / 8 / 10 / CONH2 / CSNH2 / CN / alkylcarbonyl<(1-8) > / alkoxycarbonyl<(1-8) > / alkylaminosulfonyl<(1-8) > / alkyl<(1-8) > (SO (1-) G3) / alkoxy<(1-8) > (SR alkoxycarbonyl<(1-8) > (SO)) / OCH2Ph (SO) / aryloxy<(6-10) > (SO) / heteroaryloxy<EC (1-4) Q (0-) N (0-) O (0-) S (0) OTHERQ> (SO)

19----G5

G3 = F / Cl / Br / I / R G4 = F / Cl / Br / I G5 = alkyl<(1-8)> (SO) / Cb<EC (3-8) C, AR (0)> (SO) / aryl<(6-10)> (SO) / heteroaryl<EC (1-4) Q (0-) N (0-) O (0-) S (0) OTHERQ> (SO) G6 = H / F / Cl / Br / I / NO2 G7 = H / OH / SH / NH2 / 17 / Me / Ak<EC (1-) C, BD (0-) D (0-) T> (SO (1-3) G9) / F / Cl / Br / I / NO2 / CN / (SC 303 / OMe)

198-G2 303-G27

G8 = 0 / S / NH / 19

29----G5

$$27^{14}$$
 28^{14} 28^{14} 29^{14} $29^{$

G11 = H / alkyl < (1-8) > (SO (1-) G4) / alkenyl < (2-8) > /alkynyl<(2-8)> / NH2 / alkyl<(1-8)> (SR alkoxy<(1-8)>) /COMe / alkoxycarbonylamino<(1-8)> / alkylcarbonylamino<(1-8)> / alkoxycarbonyl<(1-8)> / (SC Me) = alkyl < (1-8) > (SO (1-) G4) / (SC CF3)G12 = H / F / Cl / Br / I / NO2 / NH2 / G13 alkylamino<(1-8)>(SO(1-)G4)/CN/CONH2= 0 / S / NHG14 G15 = N / CH= NH2 / OH / SH / CHO / CO2H / CN / G16 alkylcarbonyl<(1-8)> / arylcarbonyl<(6-10)> / N3 / 242 / Hy < EC (4-8) A (1-) Q (1-) N, AN (1) N > / 258 /

Ak<BD (0-) D (0-) T> (SO (1-) G25) / NO2 / (SC 305)

$$2^{\frac{1}{4}}^{7-G18}$$
 G^{24} G^{23} G^{25} G^{29}

$$G17 = NH / 244 / O / S$$

244-G18

G19 = Cb<EC (3-8) C, AR (0)> (SO) / aryl<(6-10)> (SO) / heteroaryl<EC (1-4) Q (0-) N (0-) O (0-) S (0) OTHERQ> (SO) / 248 / alkylthio<(1-8)> (SO) / arylthio<(6-10)> (SO) / NH2 (SO) / 253

```
G20
       = aryl < (6-10) > (SO)
G21
       = alkyl < (1-8) > (SO) / aryl < (6-10) > (SO) /
         heteroaryl<EC (1-4) Q (0-) N (0-) O (0-) S (0) OTHERQ> (SO)
       = alkoxy<(1-8)> (SO) / aryl<(6-10)> (SO)
G22
       = alkyl<(1-8)>(SO(1-)G4) / dialkylamino<(1-8)> /
G23
         aryl<(6-10)> (SO) / heteroaryl<EC (1-4) Q (0-) N (0-) O (0-)
         S (0) OTHERQ> (SO)
       = H / F / Cl / Br / I / alkyl < (1-8) > (SO (1-) G4) /
G24
         dialkylamino<(1-8)>/aryl<(6-10)>(SO)/
         heteroary1<EC (1-4) Q (0-) N (0-) O (0-) S (0) OTHERQ> (SO)
       = CO2H / R / NH2 (SO) / Cb < EC (3-8) C, AR (0) > (SO) /
G25
         Hy<EC (3-8) A (1-4) Q (0-) N (0-) O (0-) S (0) OTHERQ,
         AR (0) > (SO) / alkylsulfonyl<(1-8) > (SO) /
         arylsulfonyl<(6-10)> (SO) / CH2Ph (SO) / aryl<(6-10)> (SO) /
         heteroaryl<EC (1-4) Q (0-) N (0-) O (0-) S (0) OTHERQ> (SO) /
         alkylcarbonyl<(1-8)> (SO) / alkenylcarbonyl<(2-8)> (SO) /
         alkynylcarbonyl<(2-8)>(SO) / 262 / 264 / 267
 26,0).G19
               -G20 2640)·C(0)-G22
G27
       = alkyl < (1-8) > (SO (1-) G28) /
         alkenyl<(2-8)>(SO(1-)G28)/alkynyl<(2-8)>(SO(1-)G28)
       = F / Cl / Br / I / CN / NO2 / NH2 / CO2H
G28
       = CO2H / alkyl < (1-8) > (SO) / alkenyl < (2-8) > (SO) /
G29
         alkyny1<(2-8)>(SO) / NH2(SO) /
         Cb<EC (3-8) C, AR (0)> (SO) / Hy<EC (3-8) A (1-4) Q (0-)
         N (0-) O (0-) S (0) OTHERQ, AR (0) > (SO) /
         alkylsulfonyl<(1-8)> (SO) / arylsulfonyl<(6-10)> (SO) /
         CH2Ph (SO) / aryl<(6-10)> (SO) /
         heteroaryl<EC (1-4) Q (0-) N (0-) O (0-) S (0) OTHERQ> (SO) /
         alkylcarbonyl<(1-8)>(SO) / alkenylcarbonyl<(2-8)>(SO) /
         alkynylcarbonyl<(2-8)>(SO) / 307 / 309 / 312
 3640).G19
               _G20 3C10)-C(0)-G22
DER:
         or salts
MPL:
         claim 1
         additional ring formation also claimed
NTE:
         substitution is restricted
NTE:
         also incorporates claim 14
NTE:
RE.CNT 12
              THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD
              ALL CITATIONS AVAILABLE IN THE RE FORMAT
L37 ANSWER 14 OF 25 MARPAT COPYRIGHT 2005 ACS on STN
     129:100056 MARPAT Full-text
AN
TΙ
     Anti-amyloidogenic agents
     De Guzman Mirov, Greta J.; Kelly, Jeffery W.; Lai, Zhihong; Lashuel, Hilal
IN
     A.; Peterson, Scott A.
PA
     Texas A & M University, USA
SO
     PCT Int. Appl., 68 pp.
```

CODEN: PIXXD2

DT Patent LA English FAN.CNT 1

•

PATENT NO. KIND DATE APPLICATION NO. DATE -----A2 19980702 WO 1997-US24181 19971223 WO 9827972 PI WO 9827972 A3 19990218 W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

AU 9857277 Al 19980717 AU 1998-57277 19971223

PRAI US 1996-771938 19961223 WO 1997-US24181 19971223

MSTR 1

$$G1 = OH / SH / NH2 / 11 / 56 / 79$$

$$G2 = NH / O / S / 8$$

₩**---**G3

G3 = alkyl<(1-6)>
G4 = F / Cl / Br / I / OH / alkyl<(1-8)> (SR (1-) OH) /
alkyl<(1-14)> (SO Ph) / Hy<EC (0-) N (0-) O (0-) S (2-8) C> /
Ph / alkylcarbonyl<(1-13)> (SO Ph) / 13 /
alkyl<(1-6)> (SR (1-) G10) / CH2Ph / alkenyl<(2-8)> /
cycloalkyl<(4-10)> / 22 / 29 / SO3H / PO3H2 / 33 / 35

```
= alkylene < (1-6) > (SO (1-) G19)
       = Hy < EC (0-) N (0-) O (0-) S (2-8) C > / CO2H / OH /
G6
         SH / NH2 / 15 / 18
 15(0)-0-G7 188-G7
       = alkyl<(1-8)> / Hy<EC (0-) N (0-) O (0-) S (2-8) C> /
         Ph / alkyl<(1-4)> (SR Ph)
       = 0 / s / NH / 20
G8
 2⅓----G9
G9
       = alkyl<(1-3)>
       = F / Cl / Br / I
G10
       = NH2 / 24 / 26
G11
G12
       = alkyl < (1-10) >
G13
       = alkylene<(1-4)>
G14
       = SO3H / PO3H2
G15
       = alkylene<(1-10)>
       = C(O) / R<TX "heteroatom">
G16
G17
       = H / alkyl < (1-10) >
       = F / Cl / Br / I / OH / alkyl<(1-8)> (SR (1-) OH) /
G18
         alkyl < (1-14) > (SO Ph) / Hy < EC (0-) N (0-) O (0-) S (2-8) C > /
         Ph / alkylcarbonyl<(1-13)> (SO Ph) / 43 /
         alkyl < (1-6) > (SR (1-) G10) / CH2Ph / alkenyl < (2-8) > /
         cycloalkyl<(4-10)> / 45 / 47 / SO3H / PO3H2 / 51 / 53
                     G12
47 — G12
         4<sup>6</sup>11⊕†
                                5G13-G14 5G15-G16-G17
G19
       = NH2 (SO)
       = NH / 58 / O / S / CH2 / 60 / 62 / 65
G20
 5 N --- G3 6 N --- H 6 N --- G3 G2 1 -- G2 1
G21
       = H / alkyl < (1-6) >
G22
       = (0-2) CH2
       = N / 103-1 102-80 103-91 / 105-1 106-80 105-91 /
         108-1 107-80 109-91 / 111-1 112-80 113-91 /
         114-1 115-91 114-80 / 116-1 118-91 116-80 /
         119-1 121-80 120-91 / 122-1 124-80 125-91
```

43

G24 = (1-2) CH2 MPL: claim 1

NTE: alkyl and alkenyl moieties may also be cyclic; substitution is

restricted

L37 ANSWER 15 OF 25 MARPAT COPYRIGHT 2005 ACS on STN

AN 129:69033 MARPAT Full-text

TI Multicomponent system for altering, degrading, or bleaching lignin, lignin-containing materials, or similar substances, and method for its use

IN Freudenreich, Johannes; Stohrer, Juergen; Amann, Manfred; Mueller, Robert

PA Consortium fuer Elektrochemische Industrie G.m.b.H., Germany

SO Ger. Offen., 12 pp. CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

FAN.										
	PATENT NO.			DATE	APPLICATION NO.	DATE				
						-				
PI	DE	19651099	A1	19980610	DE 1996-19651099	19961209				
	CA	2271937	AA	19980618	CA 1997-2271937	19971205				
	WO	9826127	A1	19980618	WO 1997-EP6802	19971205				
		, , ,			PL, RU, UA, US					
					FR, GB, GR, IE, IT,					
	ΑU	9855603	A1	19980703	AU 1998-55603	19971205				
	AU	719140	B2	20000504						
	ΕP	943032	A1	19990922	EP 1997-952038	19971205				
	ΕP	943032	B1	20000913						
		R: AT, DE,	ES, SE,	PT, FI						
						19971205				
		9714387				19971205				
	JΡ	2000505844	T 2	20000516	JP 1998-526185	19971205				
				20000820	RU 1999-114460	19971205				
	ΑT	196331	E	20000915	AT 1997-952038	19971205				
	ES	2150797	Т3	20001201	ES 1997-952038	19971205				
	PT	943032	${f T}$	20001229	PT 1997-952038	19971205				
PRAI	DE	1996-19651099	19961	L209						
	WO	1997-EP6802	199712	205						

MSTR 2

$$G1 \longrightarrow G1$$

$$G1 \longrightarrow G1$$

$$G1 \longrightarrow G1$$

```
= (2-) G2 / H / X / OH / SH / 36 / CHO / CN / 25 /
G1
         \mbox{CO2H} / \mbox{SO3H} / \mbox{29} / \mbox{NO2} / \mbox{14} / \mbox{31} / \mbox{Ph} (SO (1-) G4) /
         Ak < (1-5) > (SR (1-) G7) / Ak < (1-12) > (SO (1-) G4) / 38 / 16 /
         19 / PO3H2 / OPO3H2
 38----G5
       = OH / 12 / SH / NH2
G2
 1½==0
G3
       = H / OH / CHO / CN / CO2H / CONH2 / SO3H / SO2NH2 /
         NO2 / 34 / NH2 / Ph / alkyl<(1-5)> / alkoxy<(1-5)> /
         alkylcarbonyl<(1-5)>
 3½==O
       = OH / CHO / CN / CO2H / CONH2 / SO3H / SO2NH2 / NO2 /
G4
         42 / NH2 / Ph / alkyl<(1-5)> / alkoxy<(1-5)> /
         alkylcarbonyl<(1-5)>
 4½===0
G5
       = Ak < (1-5) > (SO (1-) G4)
       = Ak < (1-10) > (SO (1-) G4) / R
       = (1-) aryl (SO (1-) G4) / OH / CHO / CN / CO2H /
         CONH2 / SO3H / SO2NH2 / NO2 / 40 / NH2 / Ph /
        alkyl<(1-5)> /
         alkoxy<(1-5)> / alkylcarbonyl<(1-5)>
 4 N ===0
DER:
         and tautomers, salts, ethers or esters
MPL:
         claim 1
NTE:
         additional ring formation also claimed
    ANSWER 16 OF 25 MARPAT COPYRIGHT 2005 ACS on STN
L37
AN
    128:295176 MARPAT Full-text
TI
    Preparation of monomers useful in the production of liquid-crystalline
    polymers
    Gailberger, Michael; Strelzyk, Katja; Grundig, Petra; Barth, Anne;
IN
    Dannenhauer, Fritz; Strohriegl, Peter; Stohr, Andreas
    Daimler-Benz A.-G., Germany
PA
```

 φ^{\bullet}

Ger. Offen., 10 pp.

CODEN: GWXXBX

DTPatent LA German

FAN.	CNT	1														
	PAT	TENT NO.		KIN	ND DATE	;		API	PLICA	OITA	и ио		DATE			
						-						_				
PI	DE	19643048		A1	L 1998	0423		DE	199	6-19	6430	48	19961	L018		
	ΕP	837054		A2	2 1998	0422		EP	1997	7-11	6765		19970	926		
	ΕP	837054		A3	1999	0414										
		R: AT,	BE,	CH,	DE, DK,	ES,	FR,	GB, C	GR, :	ΙΤ,	LI,	LU,	NL,	SE,	MC,	PT,
		IE,	SI,	LT,	LV, FI,	RO										
	JP	10182556		A2	2 1998	30707		JP	1991	7-32	0232		1997	1017		
	US	6049000		Α	2000	0411		US	1991	7-95	3976		1997	L020		
	US	6423865		В1	L 2002	0723		US	2000	0-51	6511		20000	301		
	US	6313326		В1	L 2001	1106		US	2000	0-52	6756		20000	316		
PRAI	DE	1996-1964	13048	19	9961018									•		
	US	1997-9539	76	199	971020											

MSTR 1

$$G5 = CH / N / 29$$

2½---0

G6 =
$$0 / 32-7 33-9 / 34-7 35-9 / C(0) / S / ethynylene / 37-7 38-9 / 39-7 40-9 / CH2 / R$$

G7 = p-C6H4 (SO) / 46-5 43-7 / arylene (SO (1-3) G15) / heteroarylene (SO (1-3) G15) / cycloalkylene<(3-10)> (SO (1-3) G15) / (EX 133-5 136-7)

$$46$$
 43 H_2C CH CH_2 CH_2

G8 = NULL / p-C6H4 / 56-6 53-8 / arylene (SO) / heteroarylene (SO (1-3) G15) / cycloalkylene<(3-10)> (SO (1-3) G15) / 57-6 61-8

G9 = O / NH G10 = p-C6H4 / 67-6 64-58 / arylene (SO (1-3) G15) / heteroarylene (SO (1-3) G15) / cycloalkylene<(3-10)> (SO (1-3) G15)

G11 = p-C6H4 / 73-58 70-60 / arylene (SO (1-3) G15) / heteroarylene (SO (1-3) G15) / cycloalkylene<(3-10)> (SO (1-3) G15)

G12 = p-C6H4 / 79-60 76-8 / arylene (SO (1-3) G15) / heteroarylene (SO (1-3) G15) / cycloalkylene<(3-10)> (SO (1-3) G15)

G13 = O / 108-57 109-59 / 110-57 111-59 / C(O) / S / ethynylene / 113-57 114-59 / 115-57 116-59 / CH2 / R<TX "linking group">

G14 = O / 118-59 119-61 / 120-59 121-61 / C(O) / S / ethynylene / 123-59 124-61 / 125-59 126-61 / CH2 / R<TX "linking group">

G15 = alkyl<(1-20)> (SO) / alkoxy<(1-20)> (SO) / alkylthio<(1-20)> (SO) / alkylcarbonyl<(1-20)> / alkoxycarbonyl<(1-20)> / 128 / OH / F / Cl / Br / I / CN / NO2 / cycloalkyl / CHO / COMe

0 128 S --- G16

G16 = alkyl < (1-20) >

MPL: claim 16

NTE: alkylene in G3 may be interrupted by oxygen atoms

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L37 ANSWER 17 OF 25 MARPAT COPYRIGHT 2005 ACS on STN

AN 128:154351 MARPAT Full-text

Preparation of 3'-, 4'-, and 5'-C-branched deoxyribonucleosides and their use for synthesis of oligonucleotides

IN Wang, Guangyi

PA ICN Pharmaceuticals, USA

SO U.S., 30 pp., Cont.-in-part of U.S. 5,681,940.

19951102

19961216

CODEN: USXXAM

DT Patent

LA English

FAN.CNT 2

r AN.	CMT	2						
	PAT	TENT NO.	KIND	DATE	AP	PLICATION NO.	DATE	
PI	US	5712378	Α	19980127	US	1995-552363	19951102	
	US	5681940	Α	19971028	US	1994-333545	19941102	
	CA	2202280	AA	19960517	CA	1995-2202280	19951102	
	CA	2202280	С	20000815				
	CA	2307311	AA	19960517	CA	1995-2307311	19951102	
	CN	1170412	Α	19980114	CN	1995-196962	19951102	
	CN	1122040	В	20030924				
	HU	77516	A2	19980528	HU	1997-2445	19951102	
	US	6191266	B1	20010220	US	1996-766991	19961216	
	US	6743902	B1	20040601	US	2000-697545	20001025	
PRAI	US	1994-333545	19941	102				
	CA	1995-2202280	19951	102				

MSTR 1

US 1995-552363 US 1996-766991

aryl<RC (2-)> (SO (1-) G13) / heteroaryl (SO (1-) G13)

= Ph (SO (1-) G13) / aryl<RC (2-)> (SO (1-) G13) / heteroaryl (SO (1-) G13) / R / (SC NH2 / 66 / 69 / 72 / CN / NO2 / N3 / X / 75 / SH / 77 / OH) / (EX CO2Et / alkylaminocarbonyl / dialkylaminocarbonyl / OCOMe / NHCOMe / NMe2 / 101 / alkoxy / alkylthio / SO2Me / CF3 / F / Cl / Br / I / OSO2C6H4Me-p / 105 / 108 / 111)

$$G3 = H / OH / 8$$

ე-----G4

19—G6

G6 =
$$R "blocking group"> / (EX 128)$$

$$G7 = O / CH2$$
 $G8 = 24 / 34 / 43 / 51 / 60$

G11 = OH / 78 / NH2 / 84 / 86

G12 = loweralkyl (SO (1-) aryl) / aryl

G13 = R / (SC NH2 / 89 / 91 / 94 / CN / NO2 / N3 / X /

97 / SH / 99 / OH) / (EX CO2Et / alkylaminocarbonyl /

dialkylaminocarbonyl / OCOMe / NHCOMe / NMe2 / 114 / alkoxy /

alkylthio / SO2Me / CF3 / F / Cl / Br / I / OSO2C6H4Me-p /

118 / 121 / 124)

$$g^{9}$$
 g^{9} g^{1} g^{9} g^{1} g^{9} g^{1} g^{9} g^{1} g^{9} g^{1} g^{9} g^{1} g^{1

G14 = alkyl MPL: claim 1

ď

NTE: substitution is restricted

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L37 ANSWER 18 OF 25 MARPAT COPYRIGHT 2005 ACS on STN

AN 126:47223 MARPAT Full-text

TI Preparation of imidazopyridine and benzimidazole derivatives as dual histamine H1 and platelet activating factor antagonists.

IN Martin, Fionna Mitchell; Floyd, Christopher David; Spavold, Zoe Marie;
Ayscough, Andrew Paul; Whittaker, Mark

PA British Biotech Pharmaceuticals Limited, UK; Martin, Fionna Mitchell; Floyd, Christopher David; Spavold, Zoe Marie; Ayscough, Andrew Paul; Whittaker, Mark

SO PCT Int. Appl., 55 pp. CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

PI

PATENT NO. KIND DATE APPLICATION NO. DATE

WO 9633997 A1 19961031 WO 1996-GB680 19960322

W: JP, US

RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE PRAI GB 1995-8748 19950428

MSTR 6

$$G3$$
 $G3$
 N
 $G6$
 $G7$
 $G5$
 $G9$
 $GH2$

٠,

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G2
       = H / alkyl < (1-6) > / alkenyl < (2-6) > / F / Cl / Br /
         I / CN / CO2H / alkoxycarbonyl<(1-6)> / CONH2 / CHO / CH2OH /
         CF3 / alkoxy<(1-6)> / alkylthio<(1-6)> /
         alkylsulfinyl<(1-6)> / alkylsulfonyl / NH2 / NHCOMe / NO2
G3
       = H / Me
       = alkyl<(1-6)> / alkenyl<(2-6)> / F / Cl / Br / I /
G4
         alkoxy<(1-6)>
G5
       = p-C6H4 (SO (1) G4)
       = H / alkyl<(1-6)> / alkenyl<(2-6)> / alkoxy<(1-6)> /
G6
         alkylthio<(1-6)> / cyclopropyl / alkyl<(1-6)> (SR OH) /
         dialkylamino<(1-6)> / alkyl<(1-6)> (SR dialkylamino<(1-6)>) /
         CF3 / (SC Me)
G7
       = NULL / 17
 ዟና----G8
G8
       = H / alkyl<(1-6)> / alkenyl<(2-6)> / alkynyl<(2-6)> /
         alkoxycarbonyl<(1-6)>/alkoxy<(1-6)>/alkylthio<(1-6)>/
         alkyl<(1-6)> (SR alkoxy<(1-6)>) /
         alkyl<(1-6)> (SR alkylthio<(1-6)>) / alkyl<(1-6)> (SR Ph) /
       = 25-15 27-20 / 38-15 45-20 / 43-15 44-20
G9
             G14 G10-G12-G10-G12-G10-G12-GH
 2610-G12-6H
G10
       = 0 / s / NH / 23
 2 Ng------G11
       = alkyl < (1-6) > / alkenyl < (2-6) > /
G11
         cycloalkyl<(3-8)>(SO(1-)alkyl<(1-6)>)/
         alkyl < (1-6) > (SR G13) / alkyl < (1-6) > (SR OH) /
         alkyl < (1-6) > (SR \ alkoxy < (1-6) >) / (SC \ Me / cyclohexyl)
G12
       = C(0) / SO2
G13
       = CO2H (SO) / CONH2 (SO)
       = H / alkyl < (1-6) > / (SC Me)
G14
       = Hy < AN (1) C, RC (1), RS (1) M3 (1) X8> /
G15
         Cb<AN (1) C, RC (1), RS (1) M3 (1) X8>
                   = 10 THEN G3
       = IF G1
CVA
         claim 18
MPL:
L37 ANSWER 19 OF 25 MARPAT COPYRIGHT 2005 ACS on STN
     125:275910 MARPAT Full-text
     Preparation of benzylpiperidines and -piperazines as muscarinic
TΙ
     antagonists
     Lowe, Derek; Chang, Wei; Kozlowski, Joseph; Berger, Joel G.; Mcquade,
IN
     Robert; Barnett, Allen; Scherlock, Margaret; Tom, Wing; Dugar, Sundeep; et
PA
     Schering Corporation, USA
     PCT Int. Appl., 152 pp.
SO
     CODEN: PIXXD2
DT
     Patent
```

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English
LA
FAN.CNT 4
    PATENT NO.
                  KIND DATE
                                      APPLICATION NO. DATE
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                                       _____
                                      WO 1996-US1532 19960216
PΙ
    WO 9626196
                  A2 19960829
                   A3 19961003
    WO 9626196
        W: AL, AM, AU, AZ, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS,
           JP, KG, KR, KZ, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL,
           RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, UZ, VN, AZ, BY, KG, KZ,
           MD, RU
        RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE,
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           NE, SN, TD, TG
                                      CA 1996-2212895 19960216
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    CA 2212895
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                                                      19960216
    AU 9649717
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                        19960911
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                        19990128
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                    A2
                        19971210
                                      EP 1996-906286 19960216
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                   B1 20040121
        R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE,
           LT, LV
                        19990126
                                       JP 1996-525703
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                   В
    AT 258170
                    E 20040215
                                      AT 1996-906286 19960216
    ES 2215190
                   T3 20041001
                                      ES 1996-906286 19960216
    ZA 9601293
                                      ZA 1996-1293
                                                     19960219
                   Α
                         19960819
    FI 9703446
                    A 19971022
                                     FI 1997-3446
                                                     19970822
PRAI US 1995-392697 19950223
    US 1995-457712
                   19950602
                  19960216
    WO 1996-US1532
 MSTR 1
           -G34—G1——G39
      = 15-7 12-9 / 21-7 18-9
G1
G2
      = N / 22
25---G3
G3
      = H / alkyl < (1-20) >
      = 26 / 186 / 188 / CH2OH / R<TX "1-5 amino acid">
265-2616 1661-640 1662-1630
```

•

G5 = 0 / S / S(0) / SO2 / 28 / 49 / 69 / 30 / 61 / 35 / 67 / 40-6 41-27 / 44-6 43-27 / 46 / 54 / CH=CH / ethynylene / NHCONH

$$2^{N}$$
 G^{9} G^{6} G^{6

$$_{4}$$
G=G10 $_{5}$ Q=CH-G14 $_{61}$ G13 $_{67}$ G13 $_{67}$ G15

G6 = alkyl<(1-20)>
G7 = C(O) / SO2
G8 = H / Ph / alkyl<(1-20)>
G9 = H / alkyl<(1-20)> / CHO /
alkylcarbonyl<(1-20)> (SO OH)

= 0 / S / 51

(SC 760)

G10

$$g_{23}$$
 g_{25} g_{17}^{25} g_{17}^{27} g_{18}^{25} g_{25}^{25} g_{18}^{25} g_{18}^{25} g_{18}^{25}

$$_{1}$$
G $_{1}$ G $_{1}$ G $_{2}$ G $_{3}$ G $_{3}$ G $_{4}$ G $_{5}$ G

G22 = 192 / 194 / 196 / 207 / 222-6 221-189 / 227 / 230 / CH=CH / ethynylene

$${}_{1} \S \frac{1}{2} {}_{G10} \quad {}_{1} \S \frac{1}{4} {}_{G15} \quad {}_{0} \underbrace{{}_{G6} \atop {}_{0} \underbrace{{}_{G3} \atop {}_{3}} \quad {}_{2} \S \underbrace{{}_{2} 2} {}_{2} \S \underbrace{{}_{10} \atop {}_{3}} \quad {}_{2} 2 \underbrace{{}_{2} 2} \underbrace{{}_{10} \atop {}_{3}} \quad {}_{2} \underbrace{{}_{2} 2} \underbrace{{}_{10} 5} \underbrace{{}_{12} 2} \underbrace{{}_{10} 5} \underbrace{{}_{12} 2} \underbrace{{}_{10} 5} \underbrace{{}_{12} 2} \underbrace{{}_{12} 2} \underbrace{{}_{10} 5} \underbrace{{}_{12} 2} \underbrace{{}_{12} 2} \underbrace{{}_{10} 5} \underbrace{{}_{12} 2} \underbrace{{}_{$$

$$392$$
 N $3G(0)G36$ $G19$ N $G19$ $G19$

G36 = alkoxy<(1-20)> / NH2 / 399 / H /
Cb<EC (6-10) C, AR (1-), BD (ALL) N, RC (1-2),
RS (1-2) E6 (0) OTHER>

G37 = CH (SO) / N

G38 = OH / alkoxy<(1-20) > / CN / NH2 / alkylamino<(1-20) > / dialkylamino<(1-20) >

alkylamino<(1-20)> / dialkylamino<(1-20)>

H / alkyl<(1-20)> (SO G40) / alkenyl<(2-15)> /

cycloalkyl<(3-12)> (SO) / cycloalkenyl<(5-8)> /

alkynyl<(2-10)> / alkylaminocarbonyl<(1-20)> /

cycloalkyl<EC (5-12) C, RC (2)> /

Hy<EC (1-) N (4-8) C, RC (2)> / alkylcarbonyl<(1-20)> /

dialkylamino<(1-20)> / 493 / 498 / 509 / 514 / 535 / 549 /

563 / 577 / 586 / pyrimidinyl / Ph (SO) / 605 / 622 / 635 /

645 / 661 / 667 / 679 / 691 / 700 / 708 / 711 / C(NH)NH2 /

719 / 725 / 737 / alkoxycarbonyl<(1-20)> / CH2OH / 715 /
(SC cyclohexyl)

$$493$$
 641 641 535 535

$$G19 G19$$
 $G19 G19$
 $G19 G19$
 $G19 G26$
 $G26$
 $G26$

G41 = 0 / S / S(0) / SO2 G42 = H / alkyl<(1-20) > / alkylcarbonyl<(1-20) > / alkoxycarbonyl<(1-20) > / CONH2 / alkylaminocarbonyl<(1-20) > / dialkylaminocarbonyl<(1-20) > / alkylsulfonyl<(1-20) > / 611

025 - G43

G43 = Cb<EC (6-10) C, AR (1-), BD (ALL) N, RC (1-2),
RS (1-2) E6 (0) OTHER>
G44 = Cb<EC (5-8) C, AN (2) C, AR (0), BD (ALL) SE,
RC (1), RS (1) M5 (1) X8> / Hy<EC (1) Q (1) O (4-6) C,
AN (2) C, AR (0), BD (ALL) SE, RC (1), RS (1) M5 (1) X7>
G46 = O / 739

7 13 9 G 4 7

G47 = OH / alkoxy<(1-20)>
G48 = cycloalky1<(3-12)> / alky1<(1-20)> / CN /
cyclohexyl / Me / CO2Me / Pr-i / 751

G49 = H / alkyl < (1-20) > (SO) / alkylthio < (1-20) > / (SC Me)G50 = CN / CO2MeG51 = alkoxy < (1-20) > / OMe

```
and pharmaceutically acceptable salts, esters and solvates
DER:
MPL:
        claim 1
NTE:
        substitution is restricted
NTE:
        additional ring formation is allowed
STE:
        or isomers
L37 ANSWER 20 OF 25 MARPAT COPYRIGHT 2005 ACS on STN
    125:115097 MARPAT Full-text
    Preparation of sugar-modified nucleosides and their use for synthesis of
    oligodeoxyribonucleotides
    Wang, Guangyi; Ramasamy, Kandasamy; Seifert, Wilfried
IN
    Icn Pharmaceuticals, USA
PA
    PCT Int. Appl., 81 pp.
    CODEN: PIXXD2
DT
    Patent
LA
    English
FAN.CNT 2
    PATENT NO.
                   KIND DATE
                                       APPLICATION NO. DATE
    _____
    WO 9614329
                   A1 19960517
                                       WO 1995-US14600 19951102
PΙ
        W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, JP, KE, KG,
            KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL,
            RO, RU, SD, SI, SK, TJ, TT, UA, US, UZ, VN
        RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
    US 5681940
                    A 19971028
                                      US 1994-333545 19941102
                     AA 19960517
                                       CA 1995-2202280 19951102
    CA 2202280
    CA 2202280
                    С
                         20000815
                        19960517
                                       CA 1995-2307311 19951102
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                                                       19951102
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    AU 690394
                    B2
                   A1 19970820
    EP 789706
                                       EP 1995-939864
                                                      19951102
        R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE
    CN 1170412
                   A 19980114
                                    CN 1995-196962
                                                      19951102
                          20030924
    CN 1122040
                     В
    HU 77516
                     A2
                         19980528
                                       HU 1997-2445
                                                        19951102
    JP 10506915
                     Т2
                          19980707
                                       JP 1996-515519
                                                        19951102
    JP 3633626
                    B2
                         20050330
                                      RU 1997-108591
                                                        19951102
    RU 2145964
                    C1 20000227
                                      PL 1995-319944
    PL 184378
                    B1 20021031
                                                        19951102
    CZ 293731
                    B6 20040714
                                       CZ 1997-1291
                                                        19951102
    HK 1007881
                    A1 20040604
                                       HK 1998-109044
                                                        19980709
PRAI US 1994-333545 19941102
    CA 1995-2202280 19951102
    WO 1995-US14600 19951102
 MSTR 1
```

3

```
= alkyl < (1-10) > (SO G10) /
G1
         alkyl<(1-10)> (SR (1-) G7) / Ph (SO G10) / Hy (SO G10) /
         (SC alkenyl<(2-10)> (SO (1-) G8) / CN / NO2 / N3 / CF3)
       = H / OH / alkoxy<(1-10)> (SO (1-) G9) / 17
G2
```

G3 = OH / R<TX "oligonucleotide"> / 49 / 15

G4 = R<TX "blocking group"> G5 = R<TX "nucleoside base"> / (EX 67 / 74 / 85 / 93 / 102)

G6 = O / S / NH / CH2 G7 = Ph (SO G10) / Hy (SO G10) / R / (SC CN / NO2 / 20 / OH / alkoxy (SO (1-) G9) / 26 / SH / 30 / 42 / CO2H / 46 / F / Cl / Br / I / SO2C6H4Me-p / N3) / (EX CO2Et / OCOMe / NHCOMe / NMe2 / 129 / SO2Me / CF3 / 108 / 113 / 116)

$$\frac{\text{H}}{\text{G}} = \frac{\text{G}}{3} =$$

G8 = Ph / Hy
G9 = Ph / Hy
G10 = R / (SC CN / NO2 / 24 / OH / alkoxy (SO (1-) G9) /
28 / SH / 32 / 38 / CO2H / 43 / F / Cl / Br / I /
SO2C6H4Me-p / N3) / (EX CO2Et / OCOMe / NHCOMe / NMe2 / 132 /
SO2Me / CF3 / 120 / 123 / 126)

$$2^{N}$$
 G_{11} 2^{N} G_{13} $G_{$

G11 = H / Me / Et / COMe / COCF3

G12 = COMe / COCF3 / alkyl / Ph / Hy / alkyl (SR (1-) G8)

G13 = H / alkyl

G14 = H / alkyl (SO (1-) G8) / Hy / Ph

```
= OH / R<TX "oligonucleotide"> / 135
G16
 19<del>5 G</del>4
MPL:
         claim 1
L37 ANSWER 21 OF 25 MARPAT COPYRIGHT 2005 ACS on STN
AN
    124:307619 MARPAT Full-text
     Nitric oxide synthase inhibitors for prevention and treatment of shock,
     hypotension, chronic rheumatism, ulcerative colitis, cerebral ischemia,
     tumor, and insulin-dependent diabetes
    Taniguchi, Naoyuki
IN
PA
     Ono Pharmaceutical Co, Japan
so
     Jpn. Kokai Tokkyo Koho, 32 pp.
     CODEN: JKXXAF
DТ
     Patent
     Japanese
LA
FAN.CNT 1
                  KIND DATE
                                         APPLICATION NO. DATE
     PATENT NO.
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                           --<del>-</del>----
                                          ______
                     ____
    JP 08041008
                                         JP 1994-197203 19940729
                     A2 19960213
PRAI JP 1994-197203 19940729
 MSTR 2
 G2 \longrightarrow G1
     = 3 / 11
G1
G2
     = NH / 9
 Ŋ----G3
      = alkyl<(1-4)> / alkenyl<(2-4)> / Ph /
G3
        alkyl<(1-4)>(SO G4)
      = OH / Ph
G4
      = NH2 / 7
G5
 G2---G3
       = alkylene<(2-3)> / (EX CH2CH2 / CH2CH2CH2)
G6
       = cycloalkyl<(4-7)> / 16 / 18 /
G7
        Hy < EC (-2) N (-1) O (-1) S, RS (0-) E4 (0-) E5 (0-) E6 (0-)
        E7 (0) OTHER> (SO (1-4) G12)
```

G15

= alkyl

```
G8
       = OH / CO2H / alkoxycarbonyl<(1-4)> / SO3H / NH2 /
         alkylamino<(1-4)> / dialkylamino<(1-4)> / alkylthio<(1-4)>
G9
       = phenylene
       = H / X / NO2 / CO2H / alkoxycarbonyl<(1-4)> / OH /
G10
         alkoxy<(1-4)> / alkylcarbonyloxy<(1-4)> / SH /
         alkylthio<(1-4)> / 37 / Ph (SR (1-) X) / alkyl<(1-4)>
 35,----C(O)-G23
G11
       = phenylene
       = X / NO2 / alkyl < (1-4) > / CO2H /
G12
         alkoxycarbonyl<(1-4)>/OH/alkoxy<(1-4)>/
         alkylcarbonyloxy<(1-4)> / SH / alkylthio<(1-4)> / 40 / Ph /
         Hy<EC (6-) C, BD (6-) N, RC (2-), RS (1-) E6>
 45----C(0)-G23
       = alkyl<(1-2)> / 48 / 21 / 23
G13
 2914-G7
                    _c____G18 ___G28__G8
           2G15-2S-
G14
       = NULL / alkylene<(1-4)> (SO (1) G25)
G15
       = NULL / alkylene<(1-8)> / 26-4 28-24
 2616-G17-2616
G16
       = alkylene<(1-4)>
G17
       = phenylene (SR (1-2) alkyl<(1-4)>)
       = NH / 30
G18
 3 N ---- G 1 9
       = alkyl<(1-4)> / alkenyl<(2-4)> / Ph /
G19
         alkyl < (1-4) > (SO G20)
       = OH / Ph
G20
       = NH2 / 33
G21
 3 G 2 2 - G 1 9
G22
       = NH / 35
 3 N ----- G1 9
```

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169-G10 16(0)-G11-G10

```
G23
      = alkyl<(1-4)>
G24
      = H / alkyl < (1-4) > / alkenyl < (2-4) > / Ph /
        alkyl < (1-4) > (SO G4)
G25
      = cycloalkyl<(4-7)> / 43 / 45 /
        Hy<EC (-2) N (-1) O (-1) S, RS (0-) E4 (0-) E5 (0-) E6 (0-)
        E7 (0) OTHER> (SO (1-4) G12)
 4G26-G10 4G(0)-G27-G10
G26
      = phenylene
G27
      = phenylene
      = alkylene<(1-12)>
G28
MPL:
        claim 1
NTE:
        substitution is restricted
L37 ANSWER 22 OF 25 MARPAT COPYRIGHT 2005 ACS on STN
    121:255405 MARPAT Full-text
    Catechol diethers as selective phosphodiesterase IV inhibitors
TТ
    Duplantier, Allen J.; Eggler, James F.; Marfat, Anthony; Masamune, Hiroko
IN
    Pfizer Inc., USA
PA
SO
    PCT Int. Appl., 159 pp.
    CODEN: PIXXD2
DT
    Patent
LA
    English
FAN.CNT 1
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                KIND DATE
                                        APPLICATION NO. DATE
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                   A1 19940609
                                      WO 1993-US10228 19931029
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RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
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                                        CA 1993-2150812 19931029
    CA 2150812
                     С
                          20021224
    CA 2400368
                        19940609
                                       CA 1993-2400368 19931029
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                    A1
                         19940622
                                        AU 1994-55396
                                                        19931029
    AU 673569
                    B2
                         19961114
               A1 19950920
B1 20030312
                                       EP 1994-900390
                                                       19931029
    EP 672031
    EP 672031
        R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE
    JP 08501318 T2 19960213
                                   JP 1994-513129 19931029
    JP 3100984
                     B2 20001023
                    A 19990525
    BR 9307570
                                       BR 1993-7570
                                                        19931029
                                                       19931029
    AT 234270
                    E 20030315
                                       AT 1994-900390
                                                       19931029
    PT 672031
                    T 20030630
                                       PT 1994-900390
                   T3 20031001
    ES 2192192
                                       ES 1994-900390 19931029
    IL 107758
                   A1 19971120
                                       IL 1993-107758
                                                      19931125
                   A 19940603
    FI 9305379
                                       FI 1993-5379
                                                       19931201
    ZA 9308978
                   A 19950601
                                                       19931201
                                       ZA 1993-8978
    HU 65928
                   A2 19940728
                                       HU 1993-3423
                                                       19931202
    CN 1094028
                   A 19941026
                                       CN 1993-112776 19931202
    NO 9502178
                   A 19950801
                                       NO 1995-2178
                                                       19950601
    US 5814651
                         19980929
                                       US 1997-872686 19970610
                    Α
PRAI US 1992-984408
                    19921202
    CA 1993-2150812 19931029
    WO 1993-US10228 19931029
    US 1993-142328 19931126
```

•?

G1 = Me / Et / 9

F26----G2

$$G10$$
 $G10$
 $G10$
 $G10$
 $G10$
 $G10$

```
G4 = F / OH / alkoxy<(1-4) > G5 = F / OH / alkoxy<(1-4) > / (1) OPh (SO (1-) G6) G6 = alkyl<(1-4) > / alkoxy<(1-4) > / X G7 = F / OH / alkoxy<(1-4) > / (1) Ph (SO (1-) G6) G8 = NH / 15 

G9 = alkyl<(1-4) > G10 = H / alkyl<(1-4) > / alkoxy<(1-4) > / X G11 = NULL / alkylene<(1-10) > (SO (1-2) G12) / 81 / 89 / alkenylene<(2-10) > (SO (1-2) G12) / phenylene (SO (1) G12) /
```

O / NH / 83 / S / 85-5 86-80 / 94-5 95-80 / 98-5 100-80

```
8 G 1 3=0
           8 ½ -----G 9
                     86148618 0<del>8</del>615=0
                                             9619<del>9</del>620 9621—623<del>1</del>622
G12
       = alkoxy<(1-4)> / CO2H / alkoxycarbonyl<(1-4)> / OH
G13
       = Ak < EC (1-10) C, BD (0-) D> (SO (1) G12)
G14
       = alkylene<(1-5)> (SO (1) G12) / 87 /
          alkenylene<(2-5)> (SO (1) G17) / phenylene (SO (1) G12)
 8916=0
G15
       = Ak < EC (6-10) C, BD (ALL) SE>
       = Ak < EC (1-5) C, BD (ALL) SE>
G16
       = alkoxy<(1-4)> / CO2H / alkoxycarbonyl<(1-4)>
G17
       = O / NH / 92 / S / phenylene (SO (1) G12)
G18
 9½----G9
       = O / NH / 107 / S / phenylene (SO (1) G12)
G19
 187-G9
       = alkylene<(1-5)>(SO(1)G12)/96/
G20
         alkenylene<(2-5)> (SO (1) G17) / phenylene (SO (1) G12)
 9616=0
G21
       = alkylene<(1-5)> (SO (1) G12) / 101 /
         alkenylene<(2-5)> (SO (1) G17) / phenylene (SO (1) G12)
 1616=0
G22
       = alkylene<(1-5)> (SO (1) G12) / 103 /
         alkenylene\langle (2-5) \rangle (SO (1) G17) / phenylene (SO (1) G12)
 1636=0
       = 0 / NH / 105 / S
G23
 185-G9
G24
       = Hy < EC (1-4) Q (-4) N (-1) O (-1) S (0) OTHERQ (1-4)
         C, AR (1-), BD (2) D, RC (1), RS (1) E5> (SO (1-3) G25) /
         159 / 163 / Hy<EC (1-4) Q (1-) N (-1) O (-1) S (0)
         OTHERQ (5-8) C, AR (1-), BD (4) D, RC (2),
         RS (1) E5 (1) E6 (0) OTHER> (SO (1-4) G25) / 126 / 176 /
         pyridyl / pyrimidinyl / Hy<EC (1-2) Q (1-2) N (0)
         OTHERQ (4-5) C, AR (1-), BD (ALL) N, RC (1), RS (1) E6>
         (SO (1-4) G25) / 183 / 194 / Ph (SO (1-5) G25) /
```

,,`

naphthyl (SO (1-7) G25) / Cb<EC (10) C, AR (1-), BD (6) N, RC (2), RS (2) E6 (0) OTHER> (SO (1-4) G25) / Hy<EC (1-4) Q (0-) N (0-) O (0-) S (0) OTHERQ (6-9) C, AR (1-), BD (6) N, RC (2), RS (2) E6 (0) OTHER> (SO (1-4) G25) / 212 / 204 / (SC 215 / 225 / 234 / 242 / 252)

$$G32$$
 $G32$
 $G31$
 $G31$

G25 = X / alkyl<(1-6) > / 109 / alkoxy<(1-4) > / 114 / 116 / NH2 (SO) / Hy<EC (1-2) Q (1-) N (0-) O (0-) S (0) OTHERQ, AN (1-) N, RC (1-2), RS (0-) E5 (0-) E6 (0) OTHER> (SO) / NO2 / OH / CN / SO3H / alkyl<(1-4) > (SR Ph) / 118 / 123

$$\frac{G^{27}}{H_{69}}$$
 C(0)-0-G26 $\frac{1}{1}$ C(0)-G28 $\frac{1}{1}$ C(0)-C28 $\frac{1}{1}$ C(0)-C2

G26 = H / R

G27 = H / alkyl < (1-4) >

G28 = OH (SO) / NHOH

G29 = C(0) / CH2 / SO2

G30 = NH2 (SO) / Hy<EC (1-2) Q (1-) N (0-) O (0-) S (0) OTHERQ, AN (1-) N, RC (1-2), RS (0-) E5 (0-) E6 (0) OTHER> (SO)

G31 = H / X / alkyl < (1-6) > / 137 / alkoxy < (1-4) > / 142 / 144 / NH2 (SO) / <math>Hy < EC (1-2) Q (1-) N (0-) O (0-) S (0)OTHERQ, AN (1-) N, RC (1-2), RS (0-) E5 (0-) E6 (0) OTHER>

(SO) / NO2 / OH / CN / SO3H / alkyl<(1-4)> (SR Ph) / 146 /Ģ27 1929-G30 146 SO2-R G32 = H / alkyl < (1-6) > / Ph (SO) / 170 /cycloalkyl<(3-7)>/alkyl<(1-4)>(SR Ph)/alkyl<(2-5)> (SR dialkylamino<(1-4)>)-C(O)-O----G27 G33 = Cb<EC (6) C, AR (1-), BD (ALL) N, RC (1), RS (1) E6> (SO (1) G25) / Hy < EC (1-2) Q (1-2) N (0) OTHERQ (4-5) C, AN (2-) C, AR (1-), BD (ALL) N, RC (1), RS (1) E6> (SO (1) G25) G34 = Cb<EC (10) C, AR (1-), BD (6) N, RC (2), RS (2) E6 (0) OTHER> (SO) / Hy < EC (1-3) Q (0-) N (0-) O (0-) S (0) OTHERQ (7-9) C, AN (1-) C, AR (1-), BD (6) N, RC (2), RS (2) E6 (0) OTHER> (SO) DER: and pharmaceutically acceptable salts MPL: claim 1 substitution is restricted NTE: STE: racemic-diastereomeric mixtures and optical isomers L37 ANSWER 23 OF 25 MARPAT COPYRIGHT 2005 ACS on STN 120:52843 MARPAT Full-text Hydroxy derivatives of cyclohexadiene and their preparation with Pseudomonas putida Blacker, Andrew John; Brown, Stephen Martin; Bowden, Martin Charles IN Zeneca Ltd., UK so PCT Int. Appl., 27 pp. CODEN: PIXXD2 DT Patent English FAN.CNT 1 PATENT NO. KIND DATE APPLICATION NO. DATE ----------_____ WO 9317994 19930916 WO 1993-GB523 19930312 **A**1 W: AT, AU, BB, BG, BR, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, US RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG AU 9336462 AU 1993-36462 19930312 **A**1 19931005 EP 1993-905577 19930312 EP 630364 **A**1 19941228 EP 630364 19970827 В1 R: DE, GB JP 07506096 JP 1993-515502 19930312 T219950706

19960416

Α

19920313

19930312

US 1994-302648

19941117

US 5508444

WO 1993-GB523

PRAI GB 1992-5505

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G16
      = H / R / (SC X / alkyl < (1-6) > / CF3 / CN / NO2 / Ph /
        48 / OH / SH / 51)
 48(0)-0-G5 566-G5
G18
      = R / (EX X / alkyl < (1-6) > / CF3 / CN / NO2 /
        Ph (SO (1-) G4) / alkoxycarbonyl<(1-10)> / OH / SH / 55 /
        CO2Me)
 5 G1 9--G5
      = 0 / s / 57
G19
 5<sup>4</sup>)——G5
G15+G16= R<TX "moiety necessary to form a ring"> /
        (SC CH=CHCH=CH (SO G18))
MPL:
        claim 19
L37 ANSWER 24 OF 25 MARPAT COPYRIGHT 2005 ACS on STN
   119:139256 MARPAT Full-text
    Preparation of substituted quinazolines as angiotensin II antagonists
IN
    Primeau, John L.; Garrick, Lloyd M.
    American Home Products Corp., USA
PA
    U.S., 18 pp.
    CODEN: USXXAM
DT
    Patent
LA English
FAN.CNT 1
    PATENT NO.
                   KIND DATE
                                       APPLICATION NO. DATE
    -----
                                        -----
                    A 19930216
                                       US 1991-782850 19911024
PΙ
    US 5187168
                    A 19930817
                                       US 1992-927032 19920806
    US 5236925
    WO 9308170
                    A1 19930429
                                        WO 1992-US8991
                                                        19921023
        W: AU, BB, BG, BR, CA, CS, FI, HU, JP, KP, KR, LK, MG, MN, MW, NO,
            PL, RO, RU, SD
        RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, SE, BF,
            BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG
                    A1 19930521 AU 1993-31227
A1 19940831 EP 1992-925018
    AU 9331227
                                                         19921023
    EP 612317
                                                         19921023
        R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, SE
                    T2 19950112 JP 1992-507898 19921023
    JP 07500344
                                        US 1993-34030
    US 5256781
                          19931026
                                                         19930322
                     Α
PRAI US 1991-782850
                    19911024
    US 1992-927032
                    19920806
    WO 1992-US8991
                   19921023
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MSTR 2

$$G16$$
 $G18$
 $G18$
 $G19$
 $G19$

$$3\sqrt{\frac{G^2}{G^2}}$$
 $3\sqrt{\frac{G^2}{3}}$ $3\sqrt{\frac{G^2}{G^2}}$ $3\sqrt{\frac{G^2}{G^$

G3 =
$$(1)$$
 aryl< $(6-12)$ > (SO $(1-)$ G4) / F / Cl / Br

$$G4 = F / Cl / Br$$

G5 = H /
$$alkyl<(1-8)>$$
 (SO $alkoxy<(1-8)>$) / $alkyl<(1-6)>$ (SR G3)

$$G6 = 40 / 42$$

$$G7 = (1-3) \text{ CH2}$$

 $G8 = 45 / 54-7 55-12 / 57-7 58-12$

G9 =
$$H / 47 / alkyl < (1-8) > / perfluoroalkyl < (1-6) > / alkyl < (1-6) > (SR G3) / 49 / 51$$

G10 =
$$alkoxy<(1-8)>$$
 / OH / F / Cl / Br / $aryl<(6-12)>$ (SO (1-) G4) / CN / NO2 / 64 / 67 / 76 / 78

G12 = 83-15 82-23 81-22 / 89-15 88-23 92-22 / 95-15 94-23 97-22 / 101-15 100-23 102-22

G13 = 106 / 112 / 117 / SO3H / 120 / 122

G14 = H / alkyl<(1-8)> (SO alkoxy<(1-8)>) /
alkyl<(1-8)> (SR OH) / perfluoroalkyl<(1-6)> /
alkyl<(1-6)> (SR G3) / CN / NO2 / 126 / 129 / 131 / 133 /
136 / F / Cl / Br / I / 138

G15 = (1-) H / alkyl<(1-8)> (SO alkoxy<(1-8)>) /
alkyl<(1-8)> (SR OH) / perfluoroalkyl<(1-6)> /
alkyl<(1-6)> (SR G3) / CN / NO2 / 141 / 144 / 146 / 148 /
151 / F / Cl / Br / I / 153

G16 = alkyl<(1-8)> (SO alkoxy<(1-8)>) /
alkyl<(1-8)> (SR OH) / perfluoroalkyl<(1-6)> /
alkyl<(1-6)> (SR G3) / H / CN / NO2 / 156 / 159 / 161 / 163 /
166 / F / Cl / Br / I / 168

G17 = CH2 (SO) / alkylidene (SO (1-) G10) G18 = O / S / 171 / 173-1 174-4

$$1^{\frac{N}{1}} \xrightarrow{G19} \quad \int_{1^{\frac{1}{3}} \frac{G14}{3}}^{G14} f_{4}$$

G19 = H / alkyl < (1-8) > / alkyl < (1-6) > (SR G3)

or pharmaceutically acceptable salts, solvates, and hydrates DER:

MPL: disclosure

substitution is restricted NTE:

L37 ANSWER 25 OF 25 MARPAT COPYRIGHT 2005 ACS on STN

AN111:232596 MARPAT Full-text

Quinoline derivatives, their use in the treatment of hypersensitive ΤI ailments, and pharmaceutical compositions containing them

IN Huang, Fu Chi; Galemmo, Robert Anthony, Jr.; Campbell, Henry Flud

Rorer International (Overseas), Inc., USA PΑ

Eur. Pat. Appl., 44 pp.

CODEN: EPXXDW

DTPatent

English LA

FAN.CNT 5

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	PA:	CENT	NO.		KIN	D DATE	A	PPLICATIO	N NO.	DATE
PI	ΕP	3153	99		A2	19890510	E	P 1988-31	0241	19881101
	ΕP	3153	99		A3	19901128				
	ΕP	315399		B1 19960110						
		R:	AT,	BE,	CH,	DE, ES, FR,	GB, GR,	IT, LI,	LU, NL	, SE
	US	4920	132		A	19900424	U	s 1987-11	6420	19871103
	WO	8904	305		A1	19890518	W	O 1988-US	3897	19881101
		W:	AU,	JP,	US					
	AU	8927	946		A1	19890601	A	U 1989-27	946	19881101
	AU	6334	75		В2	19930204				
	JP	0350	0889		Т2	19910228	J	P 1989-50	0520	19881101
	JP	0710	7053		В4	19951115				
	ΑT	1328	56		E	19960115	A'	r 1988-31	0241	19881101
	US	5059	610		A	19911022	U	s 1990-47	7896	19900420
PRAI	US	1987	-116	420	198	71103				

WO 1988-US3897 19881101

CASREACT 111:232596 os

MSTR 1

G1 =
$$0 / s / 7-1 8-3 / 9-1 10-3 / 11-1 13-3 / (sc 136-1 138-3)$$

G2 = 0 / S

= alkylene (SO aryl)

= 0 / S / S(0) / SO2 / NH / 21 / C(0) / 23-3 24-5 /25-3 26-5 / 14-3 15-5 / 16-3 17-5 / 18-3 20-5 / (SC 139-3 140-5)

$$1^{\frac{G}{4}^{7}} - 1^{\frac{G}{1}} = 1^{\frac{G}{3}} - 1^{\frac{G}{8}} = 1^{\frac{G}{3}} - 1^{\frac{G}{3}} - 1^{\frac{G}{9}} - 2^{\frac{G}{1}} = 2^{\frac{G}{1}} - 2^{\frac{G}{1}} = 2^{\frac{G}{3}} - 2^{\frac{G}{4}} = 2^{\frac{G}{3}} - 2^{\frac{G}{6}} = 2^{\frac{G}{6}$$

$$G6 = NH / 29$$

G7 =
$$O / S / S(O) / SO2 / NH / 31 / C(O) / 37-3 38-15 / 40-3 41-15$$

$$3^{N}$$
 G^{5} G^{6} G^{6} G^{6} G^{6} G^{6} G^{6}

G8 =
$$O / S / S(O) / SO2 / NH / 33 / C(O) / 43-16 44-5 / 46-16 47-5$$

G9 =
$$O / S / S(O) / SO2 / NH / 35 / C(O) / 49-18 50-20 / 52-18 53-20$$

G11 = alkenyl / cycloalkyl / aryl / OH / alkoxy / aralkyloxy / NH2 / alkylamino / dialkylamino / aralkylamino / acylamino / CONH2 / CO2H / alkoxycarbonyl / tetrazolyl / 55

(SC 141 / 151 / 159 / 160)

$$9^{\text{G}30}$$
 $9^{\text{G}24}$ 1^{Q} 1^{C} 1^{Q} $1^{\text{$

$$\frac{1}{4}$$
 Он $\frac{1}{4}$ SO₂—G20 $\frac{1}{6}$ G21

G20 = alkyl (SO
$$(1-)$$
 X) / Ph / CH2Ph

$$G21 = H / alkyl / aralkyl$$

$$G23 = H / alkyl (SO CO2H) / alkyl (SR alkoxycarbonyl) /$$

(SC CH2CH2CHMe2)

$$G24 = OH / 93 / 97 / 103$$

$$_{1} \emptyset \cancel{7} - G14 \qquad _{1} G36 \cancel{\overline{}} \cancel{$$

$$G26 = O / S / NH / 116$$

$$G27 = alkylene (SO)$$

 $_{1}\mathbf{\mathring{G}}\mathbf{\mathring{g}}\mathbf{^{6}}\mathbf{\overset{1}{T}}\mathbf{\mathring{g}}\mathbf{\mathring{g}}\mathbf{^{8}}\quad _{1}\mathbf{\mathring{g}}\mathbf{\mathring{g}}\mathbf{^{7}}\mathbf{\overset{1}{T}}\mathbf{\mathring{g}}\mathbf{\mathring{q}}\mathbf{^{6}}\quad _{1}\mathbf{\mathring{g}}\mathbf{\mathring{g}}\mathbf{\overset{2}{Z}}\mathbf{^{7}}\mathbf{\overset{-}G}\mathbf{^{2}}\mathbf{^{6}}\mathbf{\overset{1}{T}}\mathbf{\mathring{g}}\mathbf{\mathring{q}}\mathbf{^{8}}\quad _{1}\mathbf{\overset{3}{y}}\mathbf{\overset{2}{Z}}\mathbf{\overset{-}G}\mathbf{^{1}}\mathbf{^{4}}$

G30 = $0 / S / NH / 134 / alkenylene (SO) / alkylene (SO) / <math>125-5 \ 126-92 / 127-5 \ 128-92 / 129-5 \ 131-92$

 $_{1}936_{T}988$ $_{1}97_{T}986$ $_{1}937_{G}36$ $_{1}937_{G}36_{T}918$ $_{1}34_{G}34$

DER: or pharmaceutically acceptable salts

MPL: claim 1

1 100

NTE: additional ring formation specified

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